

**PCT**WORLD INTELLECTUAL PROPERTY ORGANIZATION  
International Bureau

AM

## INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

<b>(51) International Patent Classification <sup>7</sup> :</b> <b>C07K 14/705</b>	<b>A2</b>	<b>(11) International Publication Number:</b> <b>WO 00/52050</b> <b>(43) International Publication Date:</b> 8 September 2000 (08.09.00)
<b>(21) International Application Number:</b> PCT/GB00/00727 <b>(22) International Filing Date:</b> 1 March 2000 (01.03.00)  <b>(30) Priority Data:</b> 9904441.4 1 March 1999 (01.03.99) GB 9909151.4 22 April 1999 (22.04.99) GB  <b>(71) Applicant (for all designated States except US):</b> KARO BIO AB [SE/SE]; Novum, S-141 57 Huddinge (SE).  <b>(72) Inventors; and</b> <b>(75) Inventors/Applicants (for US only):</b> GILLNER, Mikael [SE/SE]; 6162 Renstiernas Gata 38, S-116 31 Stockholm (SE). GREENIDGE, Paulette [GB/GB]; 63 Vincent Road, Luton, Bedfordshire LU4 9AN (GB).  <b>(74) Agents:</b> BANNERMAN, David, Gardner et al.; Withers & Rogers, Goldings House, 2 Hays Lane, London SE1 2HW (GB).		<b>(81) Designated States:</b> AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).  <b>Published</b> <i>Without international search report and to be republished upon receipt of that report.</i>
<b>(54) Title:</b> HOMOLOGY MODELS OF THE GLUCOCORTICOID RECEPTOR  <b>(57) Abstract</b>  A method of designing a homology model of the ligand binding domain of a glucocorticoid receptor wherein the homology model may be displayed as a three-dimensional image, the method comprising: (i) providing an amino acid sequence and an x-ray crystallographic structure of the ligand binding domain of a thyroid, estrogen or progesterone receptor; (ii) modifying said x-ray crystallographic structure to take account of differences between the amino acid configuration of the ligand binding domains of the glucocorticoid receptor on the one hand and the thyroid, estrogen, or progesterone receptor on the other hand; (iii) verifying the accuracy of the homology model by comparing it with experimentally-determined binding properties of a number of ligands for the glucocorticoid receptor; and (iv) if required modifying the homology model for greater consistency with those binding properties.		

**FOR THE PURPOSES OF INFORMATION ONLY**

Codes used to identify States party to the PCT on the front pages of pamphlets publishing international applications under the PCT.

AL	Albania	ES	Spain	LS	Lesotho	SI	Slovenia
AM	Armenia	FI	Finland	LT	Lithuania	SK	Slovakia
AT	Austria	FR	France	LU	Luxembourg	SN	Senegal
AU	Australia	GA	Gabon	LV	Latvia	SZ	Swaziland
AZ	Azerbaijan	GB	United Kingdom	MC	Monaco	TD	Chad
BA	Bosnia and Herzegovina	GE	Georgia	MD	Republic of Moldova	TG	Togo
BB	Barbados	GH	Ghana	MG	Madagascar	TJ	Tajikistan
BE	Belgium	GN	Guinea	MK	The former Yugoslav Republic of Macedonia	TM	Turkmenistan
BF	Burkina Faso	GR	Greece	ML	Mali	TR	Turkey
BG	Bulgaria	HU	Hungary	MN	Mongolia	TT	Trinidad and Tobago
BJ	Benin	IE	Ireland	MR	Mauritania	UA	Ukraine
BR	Brazil	IL	Israel	MW	Malawi	UG	Uganda
BY	Belarus	IS	Iceland	MX	Mexico	US	United States of America
CA	Canada	IT	Italy	NE	Niger	UZ	Uzbekistan
CF	Central African Republic	JP	Japan	NL	Netherlands	VN	Viet Nam
CG	Congo	KE	Kenya	NO	Norway	YU	Yugoslavia
CH	Switzerland	KG	Kyrgyzstan	NZ	New Zealand	ZW	Zimbabwe
CI	Côte d'Ivoire	KP	Democratic People's Republic of Korea	PL	Poland		
CM	Cameroon	KR	Republic of Korea	PT	Portugal		
CN	China	KZ	Kazakstan	RO	Romania		
CU	Cuba	LC	Saint Lucia	RU	Russian Federation		
CZ	Czech Republic	LI	Liechtenstein	SD	Sudan		
DE	Germany	LK	Sri Lanka	SE	Sweden		
DK	Denmark	LR	Liberia	SG	Singapore		
EE	Estonia						

## HOMOLOGY MODELS OF THE GLUCOCORTICOID RECEPTOR

### INTRODUCTION

#### Technical Field

This invention relates to combined computational and chemical methods of obtaining improved homology models of the human glucocorticoid receptor and to computational methods using such models for the design of ligands that bind to the glucocorticoid receptor.

### BACKGROUND

#### Nuclear Receptors

The glucocorticoid receptor is a member of a superfamily of soluble proteins, the nuclear receptors. Unlike receptors associated with or integrated in the cell membrane the nuclear receptors reside in the cytoplasm or the cell nucleus. The members of the nuclear receptor superfamily have in common the ability to bind specifically their respective cognate ligands as well as DNA-elements. The ligands include physiologically-relevant ligands that are small molecules such as steroid hormones (androgens, oestrogen, mineralocorticoids, progestagens, and glucocorticoids), vitamins A and D, as well as pharmacologically important synthetic hormone mimetics that can act as agonists and/or antagonists. Upon ligand binding the receptor-ligand complex is able to modulate the transcription of genes that are controlled by that particular receptor's physiologic ligand. Depending on the nature of a specific target gene, it can be either up- or down-regulated via a classical mechanism that involves the interaction of the receptor-ligand complex with specific DNA-sequences upstream of target genes or by non-classical mechanisms such as protein-protein interactions between the receptor-ligand complex and other proteins involved in a signal transduction. The nuclear receptors bind DNA by means of a protein fold that contains cysteine residues coordinated to zinc atoms, the so-called zinc finger.

The zinc-finger motif has been used to identify and to clone members of the nuclear hormone receptor family. The nuclear receptors have 5 regions: the N-terminal A-B domain that contains an activation function; the DNA-binding domain; DBD(C); the hinge D; the ligand binding domain, LBD(E), and the F-domain (that is specific for the estrogen receptor). The 3D structures for the DNA-binding domains of the GR, oestrogen receptor (ER), thyroid hormone receptor (THR) and retinoic acid receptor (RAR), have earlier been determined by X-ray crystallography or NMR spectroscopy.

More recently, the 3D-structures of the ligand-LBD complexes of some nuclear receptors, (THR, RAR, ER and progesterone receptor (PR)) have been published. The overall fold of the LBD of these nuclear receptors is an anti-parallel alpha-helical sandwich. This fold does not occur in any other known protein. Therefore it has previously not been possible to homology-model nuclear receptor LBDs correctly. A prerequisite for homology modelling is that the target and template structures have a similar tertiary structure. The sequence homology between the LBD's of various nuclear hormone receptors is low to moderate (10-50%) which alone does not guarantee that the LBDs of other members of this family will share similar tertiary folds. However, all these nuclear hormone receptors share a common function (transcriptional regulation), ID organisation (vide ante; A-E(f) region organisation), and many but not all are activated by ligand (i.e. endogenous hormones). In addition the structures of the LBDs of all members of the nuclear hormone family that have been solved to date share a common fold (antiparallel alpha-helical sandwich). Taken together, this evidence suggests that other members of this family are also likely to share this fold and therefore it should be possible to create homology models for the LBDs of these nuclear hormone receptors.

The conformation of the C-terminal  $\alpha$ -helix (helix-12) in the X-ray crystallographic structure of ER- $\alpha$  complexed with raloxifene together with the PR-based GR-homology model was used to produce a GR homology model for the study of antagonist binding.

### **Glucocorticoids**



Glucocorticoids are steroid hormones that mediate some of the body's responses to stress. The primary function of glucocorticoids is to protect the organism from the potentially harmful defence mechanisms induced by different forms of stress. Two such potentially harmful stress reactions are the induction of hypoglycaemia by insulin and the inflammatory response. Increased levels of glucocorticoids will increase the blood levels of glucose as well as exerting and anti-inflammatory action.

The mobilisation of blood glucose by glucocorticoids results from their induction of gluconeogenesis primarily by the induction of key enzymes in intermediary metabolism. For instance tyrosine amino-transferase and other transaminases are induced which results in redirection of energy in the amino acid to carbohydrate metabolism. One of the key regulatory enzymes in the gluconeogenic pathway, phospho-*enol*-pyruvate carboxykinase (PEPCK), is also induced by the glucocorticoids. The mechanism of induction of these enzymes is mediated by the DNA-binding of the steroid-activated glucocorticoid receptor (GR) which results in increased transcription of the genes for these enzymes.

In contrast, the anti-inflammatory effects of glucocorticoids involve the inhibition of the expression of a large number of proteins induced within the inflammatory response cascade. Examples of such proteins are cytokines (e.g. IL-2, IL-8), enzymes (e.g. collagenase I, iNOS, cyclooxygenase-2) and adhesion molecules. The principle mechanism involved is the repression of the transcriptional activation of these genes induced by various intermediary transcriptional factors (e.g. AP-1, NF- $\kappa$ B). Glucocorticoids prevent the induction of these genes by protein-protein interaction between the steroid-activated GR and the intermediary activating transcriptional factors.

The initial step in the mechanism of action of glucocorticoids is their binding to a specific soluble cytoplasmic receptor protein, the glucocorticoid receptor (GR). Thereafter a chaperone protein, HSP 90 is released from the GR, and the hormone receptor complex translocates to the cell nucleus. GR belongs to the superfamily of nuclear receptors that have a zinc-finger DNA-binding motif. This motif enables ligand activated GR to bind to glucocorticoid response elements (GREs) situated on DNA upstream of GR-regulated genes. The transcription of those genes is then up- or down-regulated in response to the hormone. The  $K_d$  for binding of dexamethasone to GR is  $\sim 7$ nM and the natural hormone

cortisol binds with ~ 10% of that affinity. In the PR based GR model an alternative orientation of the side chain of Thr-739 is found which enables it to hydrogen bond to both the C-20 keto group and the C21b hydroxyl group. However, it is not currently known if the C-20 carbonyl contributes to affinity.

### **Homology Modelling**

Homology modelling involves the replacement of the differing amino acids in a related template protein structure in order to produce a model of the target protein structure. The basic assumption and requirement is that the template and target have a similar three-dimensional structure. The usefulness of a homology model is to be judged on the ability of such a model to explain the biochemical data for the target structure. A homology model can never be correct in all details, but it should capture one or more of the essential characteristics of the protein. Before a determination of the three-dimensional structure of the target is available the only way to evaluate a homology model is to assess its explanatory power. That the model is reasonable from a protein structure standpoint of view is not enough, since it can be very different from the target, especially if it was made from an unsuitable template. Therefore we have in the present invention tried to validate our model by checking it and refining it against as much experimentally-derived biochemical data available for the glucocorticoid receptor as possible. For the same purpose we have also docked representative glucocorticoids in the banana shaped cavity of the homology model and minimised the resultant steroid-protein complexes with molecular mechanics. The experimental binding affinities for GR obtained in this invention were correlated with the computed protein interaction energies.

The first homology model in accordance with this invention was based on the thyroid hormone receptor (THR).

TR was initially used for homology modeling of GR. Because of the higher degree of sequence homology of the LBDs of GR vs ER (26%) than with THR (13%), and because of the close similarity of the preferred ligands of ER and GR (i.e. steroids), ER will be a better template than THR and therefore ER was then used as a preferred template for GR homology modelling in the present invention. For similar reasons a progesterone receptor (PR) was also used as a preferred template for GR modelling in the present invention.

## Glucocorticoid Structure - Activity Relationships

Synthetic glucocorticoids were investigated at an early stage for their anti-inflammatory properties. The ranking order of GR binding affinities correlates well with both the metabolic and anti-inflammatory effects of glucocorticoids. A combination of experimental, QSAR and computational chemistry studies have produced the following concept of important features for ligand binding to the glucocorticoid receptor.

The C-3 and C-20 keto groups of glucocorticoids are regarded as important for binding since their reduction to hydroxyl reduces binding affinity. This has been interpreted as suggestive of hydrogen bond donors located at corresponding positions in the receptor structure. Certain pyrazolosteroids, such as deacycortivazol, bind with high affinity although they do not have the C-3 keto group. There are also steroids without the C-20 keto group that have high affinity for GR, so neither the C-3 nor the C-20 keto group appear to be absolute requirements of glucocorticoids for high affinity GR binding.

The C-11 and C-21 hydroxyl groups are likewise as important for binding, and therefore suggest the existence of complementary hydrogen bond acceptors-donors in the receptor.

The replacement of the C-11 $\beta$  hydroxyl with a keto group is detrimental to binding whereas a chlorine substituent at this position does not lead to loss of binding affinity. A C-17 *α* hydroxyl group increases affinity of glucocorticoids for the human receptor, but decreases the affinity for the rat receptor.

Hydrophobic pockets of limited size appear to exist in GR corresponding to the C-6 $\alpha$  and C-9 $\alpha$  positions of glucocorticoids, since small halogen atoms and methyl substituents here increase binding affinity, whereas bromine or methoxy substituents in the C-0 position decrease ligand binding affinity.

It may be concluded from thermodynamic analysis that the ligand binding cavity of GR is predominantly hydrophobic since the binding enthalpy decreases when the temperature increases, which indicates that the driving force for binding is hydrophobic in nature. Surface area calculations indicate that both faces of the steroid are in contact with the protein, i.e. it is completely enclosed by the binding cavity.

An important feature of GR binding is the presence of the 4,5-diene double bond in the A-ring of the steroid. A second double bond in the A-ring, the 1-2,diene, further enhances the binding affinity. This double bond causes the A-ring to tilt downwards (toward the  $\alpha$ -face of the steroid) from the main plane of the molecule. This downward bend of the A-ring was parameterized as the distance of the C-3 to C-17 carbon atoms (A- to D-ring distance) in the QSAR study of Wolff et al. It was found in that study that the shorter this distance was, the higher the affinity of the glucocorticoid was for the glucocorticoid receptor, i.e. the more bent the steroid is out of its main plane, the higher its affinity is for the glucocorticoid receptor.

Taken together, the structure-activity relationships presented above clearly indicate that the receptor imposes strict steric requirements on ligand binding.

## UTILITY OF THE INVENTION

The glucocorticoid receptor models described in this application can be used to design new glucocorticoid receptor ligand, that can be agonists and/or antagonists. Glucocorticoid receptor agonists are useful for treatment of inflammation and immunosuppressive therapy. Glucocorticoid antagonists are expected to be useful in treatment of hypertension, diabetes, obesity, glaucoma, depression, AIDS and for wound healing.

The glucocorticoid receptor models can be used in design of new glucocorticoids in various ways. De novo drug design can be carried out by identification of features in the binding site that can be important for binding with respect to shape, charge, and hydrogen bonding properties. Ligand fragments with complementary properties to receptor features can be optimised for binding, in the same manner, by replacement of ligand fragments by better ones. Both these processes can be carried out manually or with de novo drug design programs, like LUDI and LEAPFROG given the coordinates of the glucocorticoid receptor models described herein.

The models can also be used with molecular mechanics, or 3D-quantitative structure activity relationship programs to assess the protein binding affinity of virtual glucocorticoid receptor ligands in order to prioritise their synthesis.

In summary, the homology models according to the invention will be useful for electronic screening of compound databases, de novo drug design and/or prediction of binding affinities of glucocorticoid receptor ligands for glucocorticoid receptor by means of molecular mechanics scoring functions.

## BRIEF DESCRIPTION OF THE DRAWINGS

Fig 1 is a structure of a glucocorticosteroid, dexamethasone, with atom numbering.

Fig 2a is the final alignment used between the rat thyroid hormone receptor  $\alpha_1$  and  $\beta$  sequences and the glucocorticoid receptor.

Fig 2b is the final alignment used between the estrogen receptor and sequence and the glucocorticoid receptor.

Fig 3 is a ribbon drawing of the ligand binding domain of the glucocorticoid receptor with a ligand depicted as a space-filling model.

Fig 4 shows cross-sections of a glucocorticoid receptor ligand within the binding site of the glucocorticoid receptor. The van de Waals radii of the ligand atoms as well as the water-excluded surface of the glucocorticoid receptor-model is shown as dots.

Fig 5 shows a drawing of a glucocorticoid receptor ligand with its interactions, with residues in the binding site that are critical for ligand binding.

Fig 6 sequence alignment used for homology modelling of GR from ER and TR.

Fig 7 structure of eight representative glucocorticoids used for experimental GR-binding assays and correlation with their computed protein interaction energies.

Fig 8 Graphs showing the progression of the improved correlation between calculated protein-interaction energy with the experimental free binding energy; (i) molecular mechanics ligand-protein interaction energy, (ii) inclusion of terms for ligand solvation, (iii) inclusion of terms for ligand solvation and strain energy, (iv) scaling of the individual components with respect to each other by means of PLS. Triamcinolone is not included in (i);  $R^2=0.02$  if it is included.

Fig 9 (a) RasMol representation of the main interactions with dexamethasone in the GR homology model.

(b) Sketch of the main interactions with dexamethasone in the GR homology model.

Figures 10 and 10b Orthographic views of mutations in GR LBD that affect transactivation and/or ligand binding (Table 4) displayed as balls on the  $\alpha$ -carbons. The Figure being produced with RasMol.66.

Figure 11 Sequence alignment used for homology modelling of GR from PR.

Figure 12 The three dimensional coordinates of the GR model produced from ER using its X-ray crystallographic structure as a template.

Figure 13 The three dimensional coordinates of the GR model produced from PR using its X-ray crystallographic structure as a template.

Figure 14 Sequence alignment of ER and GR used for the conformation of the C-terminal-helix (helix 12) in a PR-based GR-model for the study of binding of antagonists. The three dimensional coordinates of the GR homology model using the rat TRa/T3 and human TRb/Triac crystallographic structures.

Figure 15 The three-dimensional coordinates of the GR model produced from PR using the conformation of the C-terminal  $\alpha$ -helix (helix 12) such as is in the X-ray crystallographic structure of ER- a complexed with ralofene. A GR-specific antagonist is docked into the binding site.

## **DETAILED DESCRIPTION OF THE INVENTION**

### **Homology Modelling Based on the Thyroid Receptor**

Initial multiple sequence alignments of the ligand binder nuclear receptor sequences were obtained using the Pileup program from the Genetics Computer Group at Univ. of Wisconsin program package. For semi-automated homology modelling Modeler, as supplied with Quanta96 from Molecular Simulations Inc., was used. <sup>8</sup> The homology

modelling that we performed involved the replacement of the differing amino acids in a related protein structure (the template) in order to produce a model of the target protein structure. It is essential that the template and target have a similar three-dimensional structure. In manual homology modelling the side-chain positions of the amino-acids are then refined e.g. using rotamer libraries and energy minimisation. Loops can be copied from libraries of the other protein structures, and/or simulated by molecular dynamics. If the model does not exhibit a reasonable protein structure, or if it fails to account for the available biochemical data, the alignment is revised and the model is rebuilt. This process is preferably repeated until the model cannot be further improved. Serious manual homology modelling is thus a tedious enterprise, since the placing and refinement of the side chain positions has to be redone in each modelling cycle. Semi-automated homology modelling facilitates the interactive process since it automates the manual placement and refinement of the amino-acid side-chains as well as modelling of loops. In the present invention we used the program Modeler for this purpose.<sup>15</sup>

The initial sequence alignments were obtained from multiple sequence alignments of nuclear receptors. These alignments were used for the initial runs but they were adjusted for subsequent runs in order to produce a molecular model with a reasonable protein structure that also accounted for the available scientific data. The ligand was not included in the Modeler runs. Iterative Modeler runs, using sequence alignments taking account of the known scientific data, resulted in the final alignment (Fig. 2). The overall fold of the model is shown in Fig 3. In the water-excluded surface of the model a completely enclosed banana-shaped binding cavity can be observed. This accords with calculations that have shown that glucocorticosteroids should be completely enclosed by glucocorticoid receptor, and because it is known that the glucocorticoids with high affinity for glucocorticoid receptor are more bent out of their main-plane (have a shorter A to D-ring distance) than glucocorticoid receptor-ligands with lower affinities. cortisol was manually docked as a rigid body into the glucocorticoid receptor homology model by the best possible fits of its atomic van der Waals radii to the water-excluded surface of the binding cavity (Fig 4). The amino acid residues in the cavity were mainly hydrophobic, except for two residues namely Arg-611 and Thr-739. These were located within 3Å of the 21-OH and 19-OH of cortisol, and their side chain nitrogen atoms could constitute hydrogen bonding partners.

Furthermore, the backbone carbonyl of Leu-563 was within 3Å of the 11-OH group of cortisol, and could thus be a possible hydrogen bond acceptor (Fig 5.).

A small cavity surrounded by carbonyl oxygen atoms near the C-3 of the ligand was observed. This cavity may contain water molecules. Therefore water-mediated hydrogen bonding may be involved in the binding of the C-3 carbonyl oxygen atom. Possibly cortivazol which does not have a C-3 carbonyl oxygen may displace the water molecules by its pyrazole ring which could fill the cavity, thus explaining its high binding affinity.

That C-11 chloro substituted glucocorticosteroids have similar affinities for glucocorticoid receptor as C-11 hydroxyl substituted glucocorticosteroids has been rationalized by the assumption that there exists an accessory hydrophobic pocket for such halogen substituents.<sup>3</sup> However this assumption may not be necessary, because in our model both the C-11 chloro or hydroxyl substituents may interact with a carbonyl oxygen, and carbonyl oxygens in other X-ray structures are known to interact with halogen atoms at less than the sum of their van der Waals radii. In the THR x-ray structure the ligand iodines thus interact with backbone carbonyl oxygens.<sup>5</sup>

That the binding cavity in this model is more bent than steroid makes sense in view of the classical structure-affinity relationships for glucocorticoid-steroids since it would preserve the rank order of affinities where the most bent glucocorticoid receptor-binding steroids (that have the shortest A-D ring distances) bind with the highest affinities to glucocorticoid receptor and the more planar ligands bind with lower affinities. It is known that the receptor-bound conformations of ligands frequently differ from their minimum energy conformations. It may thus be concluded that ligand binding to a receptor is a complex process where both the ligand and the binding site has to adjust for binding.

Warriar *et al*, have shown by point mutations that M565 and G567 are important for ligand specificity and binding, respectively.<sup>12</sup> In our glucocorticoid receptor model these residues are close to the binding site. Stromstedt *et al* have covalent affinity labelling with radiolabelled glucocorticoid receptor ligands and protein sequencing studies demonstrated three residues, namely Met-622, Cys-754 and Cys-656, to be in the vicinity of the binding site of the glucocorticoid receptor<sup>13</sup>. In our initial alignment two of these residues were in our glucocorticoid receptor-model in the vicinity of the ligand. We therefore improved the



alignment so that the third residue was nearer the binding site after homology modelling. However, this revision of the models did not affect the binding site. The final alignments are shown in Fig 2A and 2B.

### Homology Modelling Based on the Estrogen and Progesterone Receptors

#### Materials

[<sup>3</sup>H]TA was obtained from NEN-Dupont, unlabelled steroids from Sigma and cell culture media, fetal bovine serum and penicillin-streptomycin from Gibco-BRL.

#### Plasmids

The mammalian vector pCMVhGR, expressing the wild type hGR, was constructed by cutting out a BamHI-XbaI fragment from pUC18/ATG-NX and inserting it into pCMV4. This fragment contains the entire coding region of the human GR gene and about 400 bp of the 3'-untranslated sequence.

#### Mammalian Cell Culture and Transfection

COS-7 cells were grown in Dulbecco's modified Eagle's medium, supplemented with 10% fetal calf serum, penicillin (100 IU/mL) and streptomycin (100 µg/mL), at 37°C in a humidified atmosphere with 5% CO<sub>2</sub>. For ligand binding assays and competition assays 10 cm plates containing cells at 60-80% confluency, plated out 1-3 days before transfection, were transfected with 10-15 µg expression vector using the calcium phosphate method. Cells were incubated 48 hours after transfection before assays were performed.

#### Ligand Binding and Competition Assays

Cells were washed with and scraped in PBS and spun in a microfuge. They were then resuspended in a buffer consisting of 1mM EDTA, 20mM potassium phosphate pH 7.8, 10% glycerol, 20mM sodium molybdate and 1 mM DTT, homogenised with a glass homogenizer and the lysate was spun for 30 min at 100,000 xg at 4°C. For saturation analysis different concentrations of [<sup>3</sup>H]TA (0.2-0.7 nM) were added and for competitive

binding assays 10nM [ $^3\text{H}$ ]TA and increasing concentrations of different non-radiolabelled steroids were added. The extracts were incubated at 4°C overnight. Bound and free [ $^3\text{H}$ ]TA were then separated by gel filtration on a Nick column (Pharmacia) and the amount of [ $^3\text{H}$ ]TA bound was measured in a scintillation counter. Free [ $^3\text{H}$ ]TA was calculated as total minus bound [ $^3\text{H}$ ]TA. The level of unspecific binding was negligible as monitored by adding 200 fold excess non-radiolabelled TA to parallel incubations with the different concentrations of [ $^3\text{H}$ ]TA.

#### Homology modelling and molecular dynamics

Initial multiple sequence alignments of the ligand binding nuclear receptor sequences were obtained using the Pileup program from the GCG program package. For semi-automated homology modelling, Modeler, as supplied with Quanta96, was run using the no optimism option, with the ER- $\alpha$  LBD/estradiol complex X-ray crystallographic structure (Brookhaven PDB accession number 1ERE) as the template. Hydrogen atoms were added to the homology model using the HBUILD routine in CHARMM. Sodium and chloride counterions were placed at the maxima and minima of the protein electrostatic potential near charged amino acid residues so as to achieve net neutrality of the system. The C- and N-termini were made neutral. The 3D molecular editor of QUANTA96 was used to build the various glucocorticoids. The constructed glucocorticoids were minimised *in vacuo* using Gasteiger - Huckel charges and a dielectric constant of 78. Partial atomic charges for the resulting structures were calculated by fitting the water-accessible surfaces of the molecules to their 6-31G\* electrostatic potentials according to Singh and Kollamn, as implemented in Gaussian 94. The 6-31G\* ESP charges were used for the ensuing protein-ligand interaction studies. The fit of dexamethasone in the binding site with the lowest ligand-protein interaction energy after minimization of various explored alternative starting orientations was chosen as an initial conformation for subsequent molecular dynamics. The minimisation was carried out with CHARMM and started with 200 initial cycles of steepest descent and continued by the adopted-basis Newton-Raphson algorithm until the root means square energy gradient was less than 0.01 kcal/Å. The default heuristic non-bonded list-update method and a distance dependent dielectric function (scaled with 1/r) were used. The protein-ligand interaction energies were when required calculated for each resulting minimised conformation. The system was subjected to molecular dynamics

using the Verlet and Shake algorithms using the same conditions as for the minimisation. The protein was surrounded by a 21 Å solvent cap of TIP3 waters centred on the ligand for the dynamics simulation. The initial dynamics simulation was for 10 ps using a step-size of 0.01 followed by 60 ps with a step-size of 0.02. The solvent cap was then removed and the remaining dexamethasone-GR complex structure resulting from the final trajectory after 70 ps of dynamics, was energy-minimised using the same constraints as described above and thereafter used for energy-minimisation with other ligands instead of dexamethasone.

The Modeler program was used, and it has been shown that it produces results as good as manual modelling at different levels of homology.

The initial sequence alignments were obtained from multiple sequence alignments of nuclear receptors. These alignments were used for the initial runs but they were adjusted for subsequent runs in order to produce a molecular model with a reasonable protein structure that also accounted for the available scientific data. The ligand was not included in the Modeler runs. Iterative Modeler runs, using sequence alignments considering the scientific data, resulted in the final alignment (Fig. 6). In the water-excluded surface of the model a completely enclosed banana-shaped binding cavity could be observed. This is reassuring, since it has been calculated that glucocorticoids should be completely enclosed by GR, and because it is known that the glucocorticoids with high affinity for GR are more bent out of their main plane (have a short A- to D-ring distance) than GR ligand with lower affinities. Dexamethasone was manually docked as a rigid body into the GR receptor homology model by the best possible fits of its atomic van der Waals radii to the water-excluded surface of the binding cavity. The initially selected position of dexamethasone within the homology model correspond to that of estradiol in the ER- $\alpha$  crystallographic complex (binding mode 1, Table 1). The dexamethasone molecule was also rotated 180 degrees about its long axis, such that the positions of the A- and D-rings were reversed (binding mode 5, Table 1) and thereafter at each of these two orientations, the molecule was rotated in steps 90 degrees about its short axis (binding modes 2-4 and 6-8, Table 1). An alternative orientation of the C-17-side chain corresponding to binding mode 1 was also investigated (binding mode 9, Table 1). The orientation with the most favourable protein ligand-interaction energy (Table 1) agrees with that of the ligand in the ER and PR X-ray crystallographic structures but not with the orientation of the

glucocorticoid in an earlier published GR model. The fit with the lowest ligand-protein interaction energy was chosen as a starting conformation for subsequent molecular dynamics. A water molecule was placed in the cavity near the C-3 carbonyl oxygen, based on the bridging water between the glutamate, arginine and 3'-OH of estradiol in the ER- $\alpha$  X-ray crystallographic structure. Side-chains of residues or water molecules within 5 Å of the ligand were allowed to move freely, whereas the main chain C, Ca and N atoms within the same zone were restrained with a harmonic potential of 100 kcal/Å. The rest of the protein was kept rigid. These restraints were imposed because too much unrestrained minimisation and molecular dynamics has in blind tests been shown to cause the homology models to be more off the target than the template. The system was equilibrated with molecular dynamics together with the explicit solvent for 70 ps. The potential energy and temperature appeared stable during the last 10 ps of the trajectory. The solvent water was then removed and the remaining dexamethasone-GR complex structure resulting from the final trajectory after 70 ps of dynamics was energy-minimised using the same constraints as described above. The other ligand structures were then fit into the binding site in this same position and orientation as the best fit obtained for dexamethasone, and energy-minimised and used for correlation with the in this study experimentally determined IC<sub>50s</sub> for human GR (Table 2).

Because a crystallographic structure of the progesterone receptor bound to an PR antagonist such as RU-38486 is not currently available, it is not certain how the conformation of PR changes when complexed with an PR antagonist. If RU-486 is docked into the binding cavity of the PR crystallographic structure or the GR homology model in an orientation analogous to progesterone in PR, there is insufficient space to accommodate its bulky 11-N,N-dimethylaniline substituent (i.e., it sterically clashes with helix-12). Therefore it is likely that H12 of GR is displaced by RU-486 in analogy to the displacement of H12 by ER antagonists in estrogen receptor complexes. This displacement of H12 will then allow sufficient space to accommodate the 11-b-substituent of RU-486 and other GR antagonists with bulky 11-b-substituents. Therefore to produce an antagonistic GR homology model, H12 and the loop connect H11 and H12 in the PR based GR homology model was moved to where it is located in the ER -raloxifene complex by superimposition of the C-carbons according to the alignment in Fig 9. This was accomplished by splicing H12 and the loop between H11 and H12 from the ER -raloxifene complex X-ray crystallographic structure

into the GR-model, followed by mutation of the ER amino acid residues to the corresponding GR residues.

Table 1 Molecular Mechanics Interaction Energies For Various Biding Modes of Dexamethasone

Binding Mode *	Molecular Mechanics Interaction Energy (kcal/mol)
1	-82.5
2	-54.4
3	-73.6
4	-57
5	-64.9
6	-73.4
7	-64.2
8	-64.2
9	-79.6

\*Binding mode 1 corresponds to that of estradiol in the ER- $\alpha$  crystallographic complex. Rotating the dexamethasone molecule in this binding mode by 180 degrees about its long axis, such that the positions of the A and D rings are reversed, results in binding mode 5. Binding modes 2-4 and 6-8 respectively, result from the progressive rotation of the molecule in steps of 90 degrees about its short axis at each of these two orientations. Binding modes 1 and 9 have a different orientation of the C-17 side.

#### Calculation of Solvation Energy

6-31G\* electrostatic potential-fit charges and the corresponding CHARMM *in vacuo* optimised geometries of the steroids were used for calculation of solvent free energies with the GB/SA algorithm as implemented in the solvation module of the pseudoreceptor drug design software package PrGen. All calculations were run on Silicon Graphics R10000 workstations under IRIX 6.2/6.4.

#### Statistical Analysis

The sigmoidal dose-response curves obtained by competitive ligand binding assays were linearized with the log-logit function and the  $IC_{50}$  determined as the intersection with the X-axis (where logit=0) as described by Rodbard. The statistical analyses were performed using Microsoft Excel 5.0 and the partial least squares methodology as implemented in the QSAR module of Sybyl 6.4.

### Molecular Mechanics Interaction Energies

Initially, the last frame of the molecular dynamics simulation performed with dexamethasone was energy minimised as described in Methods. It was noted that Thr-739 could possibly form a hydrogen bond with the steroid's 21-hydroxyl group by simple rotation of the amino acid's side-chain. The complex was then re-minimised following this alteration. As this led to an improvement in the protein-ligand interaction energy, and the 21-hydroxyl is known to contribute to the affinity of glucocorticoid steroids, this complex was then used as a template to investigate the interactions of the other ligands with the protein. A spectrum of ligands was chosen to represent typical glucocorticoids ranging from natural ligand cortisol to potent synthetic ligands such as triamcinolone acetonide. The ligands were selected to include various combinations of common substituents of pharmacologically interesting GR-ligands such as  $\Delta$ -1, 9 $\alpha$ -fluoro and 16 $\alpha$ -, 17 $\alpha$ -substitutions (c.f. Fig 7 for the structures of the ligands used in the present study).

Table 2

Table 2. Relative binding of glucocorticoids to human GR.

Ligand	$IC_{50} \pm SD^a (nM)$
Dessonide	$7.0 \pm 3.4$
9 $\alpha$ -F prednisolone	$7.3 \pm 7.0$
TA	$7.2 \pm 1.8$
Dexamethasone	$12.5 \pm 7.1$
9 $\alpha$ -F cortisol	$18 \pm 1.7$
Prednisolone	$18.4 \pm 8.5$
Cortisol	$68.0 \pm 39.5$
Triamcinolone	$131.0 \pm 7$

<sup>a</sup>n=3 for all compounds except for Ta where n=2

As can be seen from Table 2, the modifications of the cortisol structure employed here lead to quite significant alterations in binding affinity. Thus, this series of steroid ligands was well suited to challenge the explanatory powers of the model. Different orientations of the side chains of both ligands and amino acid residues were investigated and the model yielding the best correlation between molecular mechanics interaction energy and experimental data is analysed below and its interactions discussed with respect to the points described in the introduction.

It was not possible to obtain a useful correlation between the molecular mechanics interaction energy and the experimental free binding energy for all ligands (data now shown;  $R^2=0.10$  vs.  $0.45$  when triamcinolone is excluded). Triamcinolone, which is the outlier, is the only ligand in this investigation having a  $16\alpha$ -hydroxyl substituent. In other studies, it has been shown that in order to reproduce experimental relative free energies of binding, ligand desolvation effects have to be taken into account. The GB/SA algorithm has been validated with a series of small substituted hydrocarbons. We have within the context of another study (Carlsson et al., manuscript in preparation) applied the PrGen solvation module to the Wolfenden data set which consists of the experimentally determined free energies of solvation in water of ten aromatic and cyclic molecules. Due to the greater degree of resemblance of the molecules in the Wolfenden data set to drug molecules, the solvation energies calculated by the solvation module of PrGen are scaled according to the equation resulting from the fit between that data set and the experimental data

$$(\Delta G_{\text{solv}}(\text{GB/SA}) = (\Delta G_{\text{solv}}(\text{PrGen}) + 0.25) / 0.88; R^2 = 0.91$$

with 6-31G\* ESP charges calculated on the CHARMM in vacuo optimised geometries.

When a solvation correlation was included, the correlation between computed and experimental free energies for GR ligand binding was not improved ( $R^2 = 0.01$  for all ligands vs.  $0.45$  when triamcinolone is excluded). The activity of triamcinolone was under-predicted in the correlation, as its C-15 $\alpha$ -hydroxyl group was unable to make any hydrogen bonds with the protein but yet had the largest solvation penalty (Table 3). It was

then noted that Gln-642 could make a hydrogen bond with the C-16 $\alpha$  hydroxyl oxygen atom of triamcinolone and the C-16 ether oxygen atoms.



Table 3: Summary of Ligand-Protein Interaction Energies (kcal/mol), Calculated Solvation Energies (kcal/mol), Ligand Strain Energies (kcal/mol) and Experimental Binding Affinities (kcal/mol) of the Glucocorticoids.

Ligand	Molecular Mechanics Interaction Energy (kcal/mol)	Scaled Calculated Solvation Energy (kcal/mol)	Ligand Strain Energy (kcal/mol)	Experimental free binding energy <sup>a</sup> (kcal/mol)	$-\Delta G_{\text{bind (exptl.)}}$
Desonide	-78.0	-26.32	5.66	11.55	
9 $\alpha$ -F prednisolone	-72.4	-23.33	3.08	11.53	
TA	-78.7	-25.88	5.96	11.47	
Dexamethasone	-74.3	-21.13	4.71	11.24	
9 $\alpha$ -F cortisol	-72.1	-20.35	3.42	11.04	
Prednisolone	-73.9	-21.81	2.90	11.03	
Cortisol	-70.6	-17.99	2.93	10.32	
Triamcinolone	-82.9	-27.78	5.69	9.96	

<sup>a</sup>  $\Delta G_{\text{bind (exptl.)}} = RT \ln K^*$ ,  $K^* = (1/K_d \text{ for } [^3\text{H}]\text{TA}) / (\text{IC}_{50} \text{ for tested ligand} / \text{IC}_{50} \text{ unlabeled TA})$ ,  $K_d$  for TA = 0.66 nM.

of triamcinolone acetonide and desonide. Thus, the side chain of Gln-642 was rotated so as to achieve a hydrogen bond with the C16-oxygen substituent of these ligands and the complexes minimized. Although the other steroids do not possess a C16-substituent capable of acting as either a hydrogen bond donor or acceptor, Gln-642 in these complexes was also rotated to the same position as that in triamcinolone and the resulting complexes minimised. The amide nitrogen of Gln-642 formed hydrogen bonds ( $\sim 3.1\text{\AA}$ ) with the S of Met-639 and also with the 16 $\alpha$  oxygen atoms of triamcinolone, desonide and triamcinolone acetonide. A good correlation between the molecular mechanics interaction energy for all the ligands could then be achieved with this model if solvation and ligand strain energy (ligand strain energy is the difference in energy between the ligand conformation in the protein and when minimised in vacuo) corrections were included. Figure 8 shows the progressive improvement of the correlation with the addition of these corrections. the  $R^2$  increases from 0.04 (0.49 without triamcinolone; Fig 8A) to 0.48 with the solvation penalty (Fig 8B) and further to 0.69 if the ligand strain energy penalty is also included (Fig 8C). When considering only molecular mechanics interaction energy together with ligand strain energy, the correlation coefficient is 0.1 (0.49 without triamcinolone). Thus it is the combination of the solvation and strain terms that results in good correlation with the experimental free energy binding data. A partial least squares analysis using the molecular mechanics interaction energy together with the solvation (not scaled according to Wolfenden data set) and strain energies was then performed, increasing the  $R^2$  from 0.04 (molecular mechanics term only) to 0.80 (inclusion of solvation and strain energies, Fig. 3(iv)). The resulting equation was:

$$\Delta G_{\text{bind}}(\text{calc}) = 0.384 - \Delta G_{\text{inter}}(\text{MM}) 0.343 - \Delta G_{\text{solv}}(\text{PrGen}) - 0.466 - \Delta G_{\text{strain}}(\text{MM}) - 31.058.$$

The main interactions of dexamethasone with the protein are shown schematically in Fig. 4. In another model the C-17-side-chain of the ligands was rotated so as to enable the C20-keto group to form a hydrogen bond with the CD2 hydrogen of Tyr-735, but at the same time maintaining the hydrogen bond interaction between the C21-hydroxyl and Thr-739. Such hydrogen bond interactions have been reported in the literature and interestingly, Tyr-735 corresponds to His-524 in hER $\alpha$ , the residue which forms a hydrogen bond with the C-17-OH group of estradiol. The corresponding residue for the other members of the steroid hormone superfamily is either a phenylalanine or a tyrosine.

However, this model yielded a poor correlation ( $R^2 < 0.5$ ) and was therefore discarded from further analysis.

It will be noted that whilst the description refers to a method of designing a GR homology model from rat thyroid hormone receptors and a Human Progesterone Receptor, the same process may be used to design a GR model from a Human Progesterone Receptor. Figure 11 shows the sequence alignment which would be used to design a GR from PR.

### **Explanation of the Glucocorticoids Structure-Activity Relationships**

#### Reduction of the C-3 keto to a hydroxyl group reduces binding affinity

Tanenbaum et al have contrasted the hydrogen bonding interactions of the phenolic group of estradiol and the C-3 keto group of progesterone complexed with their respective receptors. Steroid receptors which bind 3-keto groups have a conserved glutamine corresponding to the sequence position of Gln-725 in hPR, but the equivalent residue in hER $\alpha$  is a glutamate residue (Glu-353). Hence, these residues are responsible for the discrimination by the steroid receptors of keto and hydroxy moieties as the arginine residues which form either direct (hPR) or direct and water mediated interactions (hER $\alpha$ ) with the keto and hydroxyl functions are conserved throughout the steroid receptor family. Additionally, there is a conformational change (atomic displacement) associated with a change in hybridization from a  $sp^2$ C-3 keto to a  $sp^3$  hydroxyl. Thus, as the ligand makes several hydrogen bonds with the receptor, a protein with functional groups at an optimum separation for simultaneous binding to the O-3 and O-20 keto oxygen atoms, and O-11, O-17 and O-21 hydroxyl oxygen atoms may bind less to a ligand which has a 3-hydroxyl group instead of a 3-keto group.

In our homology model, the C-3 keto groups of the glucocorticoid ligands form direct hydrogen bonds with Gln-570 and Arg-611. In contrast, in hPR Arg-766 directly contacts progesterone's C-3-keto group, and in hER $\alpha$  the equivalent interaction (Arg-394) with the phenolic oxygen of estradiol is also direct.

#### Reduction of the C-20 keto group reduces binding affinity

In the homology model, the C-20 keto group does not engage in hydrogen bonding, but does have a favourable electrostatic interaction with the sulfur of Met-560. For the eight glucocorticoids, the O-A distance is  $\sim 3\text{\AA}$ . (Many examples of both intermolecular and intramolecular nonbonded sulfur-nucleophile close contacts in which the sulfur-nucleophile distance is less than the sum of the sulfur and nucleophile van de Waals radii have been reported in the crystallographic literature).

The C-11 $\beta$ - and C-21 $\beta$ - hydroxyl groups are important for binding

The main weakness of the present model is its inability to explain the importance of the C-11 $\beta$ -hydroxyl as the nearest potential hydrogen bond partner is the backbone carbonyl of Leu-563, with a distance of  $\sim 4\text{\AA}$ . That C-11 $\beta$ -chloro substituted glucocorticoids have similar affinities for GR as C-11 $\beta$ -hydroxyl substituted glucocorticoids has been rationalised by the assumption that there exists an accessory hydrophobic pocket for such halogen substituents. However this assumption may not be necessary, because in our model both the C-11 chloro or hydroxyl substituents may interact with the Leu-563 carbonyl oxygen, and carbonyl oxygens in other X-ray structures are known to interact with halogen atoms at less than the sum of their van de Waals radii. In the thyroid hormone receptor X-ray structure the ligand iodines interact thus with backbone carbonyl oxygens.

The C-21 hydroxyl forms a hydrogen bond ( $2.6\text{\AA}$ ) with Try-739 and also with the backbone carbonyl of Tyr-735 ( $2.9\text{\AA}$ ). Thr-730 corresponds to Thr-894 in hPR, but in the complex with progesterone (which lacks the C-21 hydroxyl group) no hydrogen bond could be made by this residue with the ligand.

A C-17 $\alpha$  hydroxyl group increases affinity for the hGR, but decreases it for rat GR

The C-17 $\alpha$  hydroxyl group in both cortisol and 9 $\alpha$ -F cortisol forms a good hydrogen bond with Met-639 (oxygen-sulfur distance =  $\sim 3.2\text{\AA}$ ). However, from our model it appears that compounds possessing a 16-methyl substituent are unable to form a short hydrogen bond with this residue due to a steric repulsion between Met-639 and 16-Me. By comparing the sequences of rat and human GR, there were no species differences in the vicinity of Met-639. Thus the model is unable to explain the intolerance of the rat GR for a C17 $\alpha$ -OH group.

Bromine or methoxy substituents in the C-9 position decrease ligand binding affinity

The C-9a fluorine of the ligands is in close contact with the CE2 carbon atom of Phe-623 (3.4Å). Thus, introducing a more bulky substituent would presumably result in the displacement of Phe-623 from a position in which it can form a "pi-teeing" interaction with the ligand's A-ring and/or displacement of the ligand from its preferred position, causing a disruption of its interactions with the receptor.

The ligand is completely enclosed by the hydrophobic binding cavity

In the model the ligand is completely enclosed by predominantly hydrophobic residues: Leu-563, Leu-566, Trp-600, Met-601, Met-604, Phe-623, Leu-723 and Leu-753. The ligands make many favourable hydrophobic contacts with the receptor, in particular the C18- and C19- methyl groups with Met-601 and Leu-732 respectively. Significantly, these residues are preserved in the hPR, human androgen receptor and human mineralocorticoid receptor, whose ligands also have C18- and C19- methyl groups, but not in hER whose natural ligands 17  $\beta$ -estradiol lacks the C19-methyl group. Additionally, hydrophobic contact exist between the C16-methyl group of dexamethasone and the acetonide functions of desonide and triamcinolone acetonide with Tyr-735.

In order to assess the utility of the PR-based GR homology model modified to accommodate GR antagonists for the design of such drugs the compound 10e described Gebhard et al. Biorg. Med. Chem. Lett. 7(17) 2229, 1997 was used. The ligand was placed in the receptor with its steroid core in the same orientation as progesterone in PR and the complex minimized to gradient norm of 0.05 with the residues within 7 Å of the ligand treated as flexible while the remainder of the protein was held rigid. After minimization the carbonyl oxygen atom of the 2-oxo-1-pyrrolidinyl group was within hydrogen bonding distance (2.7 Å) to the hydroxyl oxygen atom of Thr-556, which corresponds to Ser-711 in PR. The distance from the steroid C-3 carbonyl oxygen atom to Arg-611 was 2.6 Å. Thus the model may be used to interpret and improve the binding of GR antagonists to GR.

A second double bond in the A-ring improves binding affinity

The fact that the binding cavity in this GR homology model is more bent than the steroid ligand is consistent with the classical structure-affinity relationship for glucocorticoids, since it would preserve the rank order of affinities where the most bent GR-binding steroids (those that have the shortest A- to D- ring distances) bind with the highest affinities to GR and the more planar ligands bind with lower affinities. It is known that the receptor bound conformation of ligands frequently differs from the minimum energy conformation of ligands. In the liganded RAR structure the 9-cis retinoic acid is more bent than the binding cavity whereas the all-trans retinoic acid is flatter than the binding cavity. It was thus concluded that ligand binding to a nuclear receptor is a complex process where both the ligand and the binding site have to adjust for binding. If our modelling has produced a correct impression of the ligand binding cavity, the above statement will be valid for GR as well.

Each of the pair cortisol and prednisolone, 9 $\alpha$ -F, prednisolone represent ligands which differ only in whether they have a 1,2-diene double bond or not (Fig 7). In our model, the A-ring of the 1,2-unsaturated ligands adopt a 1 $\alpha$ , 2 $\beta$ -half chair conformation which represents one of the ideal forms. Relative to the docked 9 $\alpha$ -F prednisolone, the 3-C keto oxygen of the docked 9 $\alpha$ -F cortisol is displaced by 0.2Å. This leads to minor adjustments in its interactions with the protein so that the coordinates of the water oxygen atom and nitrogen of the Gln-570 side-chain differ by 0.1 Å as compared to those in the 9 $\alpha$ -F prednisolone protein binding site. Additionally, displacements of the 11-O, 17-O, 20-O and 21-O oxygen atoms and 9 $\alpha$ -F atom of between 0.1 to 0.2Å occur. Atomic movements of the same magnitude also occur for cortisol with respect to prednisolone, with the exception of the 17-O and 20-O atoms which are displaced to a lesser extent, (0.04 Å vs. 0.1Å respectively). Prednisolone has a distinctly superior molecular mechanics interaction energy as compared to cortisol (~3 kcal/mol), but 9 $\alpha$ -F cortisol has only a marginally better molecular mechanics interaction energy than 9 $\alpha$ -F prednisolone (Table 3). These differences are attenuated (9 $\alpha$ -F cortisol vs 9 $\alpha$ -F prednisolone) or at least maintained (cortisol vs prednisolone) when ligand strain energy is added to the molecular mechanics

term (Table 3). Thus, the model does reflect the preference of GR for ligands with a 1,2-diene double bond relative to those that lack this feature.

The shorter the C-3 to C-17 distance the higher the affinity of a Glucocorticoid is for the Glucocorticoid Receptor

Although there is not a direct relationship between the C-3 to C-17 distance of the ligand in the homology model and ligand binding affinity (Table 4), it is notable that this distance is greatest for cortisol and its 9-fluorinated analog. When compared to the other ligands, both lack a 1,2-diene double bond in the A-ring and with the exception of triamcinolone, they have the highest free binding energies (together with prednisolone).

Explanation of Mutational Data

The HSP90 heat-shock protein is required for GR ligand binding, but as a part of activation of GR which is conceived as a steroid-induced conformation change of Gr necessary for DNA-binding and glucocorticoid dependent transcriptional regulation) it dissociates from the receptor. The HSP90 interaction sites on the GR surface have been mapped with peptide competition studies. It was found that the critical contact site is located in the region between residues 632-659 of mouse GR. In our model this region (626-653) in hGR) corresponds to S1-S2 hairpin  $\beta$ -sheets and H6-H7  $\alpha$ -helices which constitute a part of the protein surface and which also line the binding cavity. Thus, our GR model is consistent with what is known about the GR-HSP90 interactions.

A number of mutations of GR in various species have been described. Most of the mutations in the GR LBD completely disrupt the function of the receptor, presumably by perturbation of the fold of the LBD. Those detrimental mutations are not useful for validation of a GR homology mode. On the other hand, mutations in the LBD that affect ligand binding specificity and/or GR ligand-dependent activation/repression of transcription without totally activating the protein are of the greatest interest for our invention, validation of a GR homology model, since they ought to be located near the binding site. Such residues whose mutations modulate the function of GR are (in terms of the human GR sequence): P541, M565, G567, A573, M601, C638, D641, C643, M646, L653, C665, E668, V729, C736, T774, 764, F774, and these are shown as purple balls in

the receptor model in Fig. 10a and 10b. It can be seen that they seem to cluster around the ligand site and/or on H12 or its vicinity. Most of the mutations which are non-detrimental to protein activation are within 7 Å of the ligand, i.e. on the parts closest to the binding site of the helices that line the binding cavity (Table 5). Most of the mutated side-chains had direct ligand contact before the mutation (c.f. the inventory of the residues lining the binding cavity). That those mutations affect ligand binding affinity and/or ligand-dependent transactivation is thus consistent with our model.

Table 4

Summary of Ligand Binding Affinities and C-3/C-17 Distances (Å) within Homology Model

Ligand	-ΔGbind(exptl.) (kcal/mol)	C-3/C-17 (Å)
Desonide	11.55	8.21
9αF prednisolone	11.53	8.3
TA	11.47	8.24
Dexamethasone	11.24	8.28
9αF cortisol	11.04	8.45
Prednisolone	11.03	8.23
Cortisol	10.32	8.47
Triamcinolone	9.96	8.17



Table 5. Mutations affecting GR transactivation/ligand affinity within GR.

Mutation	Decreased affinity for DEX	Decreased transactivation with DEX
P541A	<i>nt</i>	> 100-fold
L563F	6-fold	15 – 60-fold
M601L	3-fold	<i>nt</i>
C638Y	Normal	Normal
C638G	10-fold INCREASED	10-fold INCREASED
C638W	Normal	Normal
D641G	Normal	no activity
D641V	Normal	no activity
C643R	<i>nt</i>	Slightly reduced
C643G	<i>nt</i>	2 – 3-fold
C643S	4-fold	<i>nt</i>
M646T	<i>nt</i>	Slightly reduced
L653S	Reduced	Reduced
C665A	<i>nt</i>	> 100-fold
C665S	<i>nt</i>	4-fold
M666I	4-fold	10 – 25-fold
E688K	Normal	no activity
V729I	2-fold	4-fold
C736S	2-fold	10-fold
C736G	<i>nt</i>	no activity
T744I	<i>nt</i>	Reduced
I747T	2-fold	50-fold
L753F	Normal	no activity
Y764N	2-fold	3 – 4-fold
F774A	6-fold	20-fold

DEX = dexamethasone

*nt* = not tested

Some mutated residues were remote from the ligand, or did not have direct ligand contact. These mutations were further scrutinised, in order to confirm that they do not invalidate our GR homology model. Mutations in residues <523 and residues >761 are in the hinge or on the C-terminal part of H12 that is not included in the template X-ray structure and outside our GR model so they cannot be used for model validation.

The P541A mutation in Gr results in that more than 100-fold increase in steroid concentration is needed to preserve biological activity, presumably due to decreased steroid affinity. Although this mutation is remove from the binding site it is at the very beginning of the strand between H1 and H3 (at the end of H1) and it may therefore be critical for its conformation. This strand (consisting of residues 540-560) delimits the binding site with residues 542-544. Therefore, a conformational change in this strand brought about by the P541A mutation could affect ligand binding from a distance.

The patient mutation V762I which reduces affinity for dexamethasone 2-fold and the C643S mutation, which reduces affinity 4-fold, are located in proximity of the ligand binding site but the side chains of the residues are not directed towards the steroid. Thus, these residues do not appear to be in direct contact with the steroid and secondary effects of these mutations would be required to explain the difference in ligand affinity. The L653S and F744A mutants that were reported by Garabedian and Yamamoto were tested in a yeast expression system, in which binding receptor binding assays were not performed so their effect may be exerted on transcription only, and need not necessarily directly affect ligand binding.

The I747T mutation reported by Roux is 9-10Å from the ligand, so it is difficult to explain why it decreases binding affinity with our model. The E688K mutation has been reported by Garabedian and Yamamoto to abolish transcriptional activity of Gr expressed in yeast and COS cells and to decrease the affinity for dexamethasone. This residue is located on H9, as far from the binding site as you can get in the GR LBD, located near H1 and facing outwards. It is here H1 connects to the hinge region to the DBD and thus it is plausible that the effect of this mutation is caused by disturbances of the interaction with DBD, rather than an direct effect on the binding site.

The C655A/S mutants required a 100-fold higher steroid concentration for biological activity of the mouse GR, but C665S in human GR has no effect on binding affinity. This residue in our model is located in H8, remove from the ligand, but since it does not affect binding affinity it does not have to be located near the binding site to validate our model. Hence, the inhibition of binding observed by Lee et al, by the mutation of the neighbouring residue, M666I, is then difficult to rationalise. However, their other mutation affecting binding affinity, L563F is near the C-ring of the steroid's  $\alpha$ -face, and thus consistent with the model.

Warriar et al, have described that the point mutations M565R and A573Q greatly enhance the affinity of Gr for dexamethasone, whereas the G567A mutant fails to bind ligands efficiently. In our GR model these residues are relatively close to the binding site. The C $\alpha$ 's of M565, G567 and A573 are  $\sim 7\text{\AA}$  from C1,  $3\text{\AA}$  from C2 to  $11\text{\AA}$  from the C3-carbonyl of dexamethasone, respectively. IN our model G567 and A574 are facing the binding cavity, in contrast to M565, which is directed from it( and constitutes part of the protein surface). Thus the M565R mutation should not affect the ligand affinity of GR to a great extent if our model is correct. In the context of another study (Lind. U., Wright, A.P.H. and Carlstedt-Duke, J., ms. in preparation) a random combination of GR to mineralocorticoid receptor mutations (between residues 565-574) was created and screened for activity with glucocorticoids and mineralocorticoids. We found in agreement with Warriar et a., that the A573Q mutant had increased activity with dexamethasone, and that the G567A mutation inactivated GR. Finally, in contrast to Warriar et al, it was also found that the M565R mutant had no effect on the activity of dexamethasone which is in better agreement with the GR model proposed.

Thus, of the mutations described in the literature affecting ligand affinity, only two (M666I, I747T) cannot easily be accounted for by the present GR-model.

Carlstedt-Duke et al have demonstrated three residues to be in the vicinity of the binding site of GR by covalent affinity labelling with radiolabelled Gr ligands with protein sequencing studies, Cys-638 is affinity-labelled through an electrophilic group of the 21-position in dexamethasone 21-mesylate reacting with a thiol. There is an absolute requirement for the C-20 carbonyl group for this labelling reaction. In our model the sulfur

of Cys-638 is located 7 Å from the hydroxyl oxygen on C-21 of dexamethasone. The Cys-736 sulfur is even closer, which may explain why this residue is preferentially labelled.

Regarding the other two affinity labels, the chemistry is not known following the photoactivation of UV-light of the bound TA ligand. In our GR-model the C-18 and C-19 methyl groups of Ta are located within 4 Å of Cys-736S, and 5.6 Å of Met-604S, respectively. If the reaction mechanism involves direct binding to the A- or B-ring, the affinity labelling of Cys-736 would require that the ligand be flipped with respect to A- and B-ring location at the time of the reaction. These two support the orientation of the steroid. In an earlier GR model the orientation of the dexamethasone is reversed with respect to the location of the A- and D-rings. With that orientation the Cys-736 is closer to the A-ring, but the other two residues (Met-604 and Cys-638) involved in the covalent affinity labelling are much further away, as compared to our orientation of the steroid. Thus, the orientation of the steroid in our model is more congruent with the affinity labelling data previously known.

Figures 12 and 13 show the X-ray crystallography data obtained from the GR models produced using the X-ray crystallographic structures of TR, ER and PR as templates.

### References

1. Muck, A.; Guyre, P.M. Glucocorticoid physiology and homeostasis in relation to anti-inflammatory actions; in *Anti-inflammatory steroid action: Basic and clinical aspects*; Academic Press: 1989, pp 30-47
2. Gronemeyer, H.; Laudet, V.; "Transcription factors 3: nuclear receptors"; *Protein Profile* 1995, 2, 1173-1308.
3. Zeelan, F.J. In *Medicinal Chemistry of Steroids*. Elsevier: Amsterdam 1990.
4. Wolff M.E.; Baxter, J.D.; Kollman, P.A.; Lee, D.L.; Kuntz, I.e.; Bloom, E.; Matulich, D.T.; Morris, J.G.N; "Nature of steroid-glucocorticoid receptor interactions: thermodynamic analysis of the binding reaction."; *Biochemistry*. 1978, 3201-3208.

5. Wagner, R.L.; Apriletti, J.W.; McGrath, M.E.; West, B.L.; Baxter, J.D.; Fletterick, R.J.; "A structural role for hormone in the thyroid hormone receptor"; Nature 1995, 378, 690-697.
6. Brzozowski AM, Pike AC, Dauter Z, Hubbard RE, Bonn T, Engstrom O, Ohman L; Greene G L, Gustafsson J A; Carlquist M.; "Molecular basis of agonism and antagonism in the oestrogen receptor Nature. 1997, 389, 753-758.
7. Bourguet W, Ruff M, Chambon P, Gronemeyer H, Moras; "Crystal structure of the RAR-gamma ligand-binding domain bound to all-trans retinoic acid." Nature 1995, 378, 377-382.

CLAIMS

1. A method of designing a homology model of the ligand binding domain of a glucocorticoid receptor wherein the homology model may be displayed as a three-dimensional image, the method comprising:

(i) providing an amino acid sequence and an x-ray crystallographic structure of the ligand binding domain of a thyroid, estrogen or progesterone receptor,

(ii) modifying said x-ray crystallographic structure to take account of differences between the amino acid configuration of the ligand binding domains of the glucocorticoid receptor on the one hand and the thyroid, estrogen, or progesterone receptor on the other hand,

(iii) verifying the accuracy of the homology model by comparing it with experimentally-determined binding properties of a number of ligands for the glucocorticoid receptor, and

(iv) if required modifying the homology model for greater consistency with those binding properties.

2. A method according to claim 1, wherein amino acids lining the binding cavity of the glucocorticoid receptor are identified chemically and the information thus gained used to verify and if appropriate modify the homology model.

3. A method according to claim 2, wherein (v) amino acids lining the binding cavity of the glucocorticoid receptor are identified by chemically mutating the glucocorticoid receptor so as to change one amino acid thereof, and experimentally determining how the

mutation affects the binding properties of the receptor to one or more ligands known to bind to the unmutated receptor.

4. A method according to claim 3, wherein step (v) is repeated one or more times, each time changing a different amino acid of the glucocorticoid receptor.
5. A method according to claim 2, including: (vi) introducing a photolabile group into a ligand having affinity for the glucocorticoid receptor, and forming a complex of the modified ligand with the receptor, expose the resulting complex to light to cause it to decompose to form reactive groups which bind to adjacent amino acids of the receptor, break up the complex into peptide fragments, analysing fragments to identify those bound to reactive groups from the modified ligand and thus the amino acids lining the binding cavity of the receptor.
6. A method according to any preceding claim, wherein the homology model is compared with the structures of other, similar, proteins.
7. A method according to any preceding claim, wherein the homology model is checked and if necessary modified to ensure that it shows predominantly hydrophobic amino acids lining the binding cavity and predominantly hydrophilic amino acids exposed to the outside.
8. A method according to any preceding claim, wherein the thyroid, estrogen or progesterone receptor is a human receptor.

9. A homology model of the ligand binding domain of a glucocorticoid receptor designed in accordance with any preceding claim and having hydrogen bonding partners for the C-16 and C-21 OH groups of a glucocorticosteroid.
10. A homology model according to claim 9, showing a hydrophilic cavity positioned to interact with the C-3 carbonyl group of a glucocorticosteroid.
11. A homology model according to claims 8, 9 or 10, showing at least one small hydrophobic pocket capable of interacting with a methyl or halogen substituent at the C-6 and/or C-9 position of a glucocorticosteroid.
12. Use of a homology model according to any of claims 9 to 11 to identify or design ligands capable of binding to the ligand binding domain of a glucocorticoid receptor.
13. Use of a homology model according to any of claims 9 to 11 to identify or design glucocorticoid receptor antagonists or agonists.
14. A glucocorticoid receptor antagonist or agonist identified by use of a homology model according to any of claims 9 to 11.
15. A medicinal product comprising a glucocorticoid agonist according to claim 14 for treatment of inflammation or for use in immunosuppressive therapy.



16. A medicinal product comprising a glucocorticoid antagonist according to claim 14 for use in the treatment of hypertension, diabetes, obesity, glaucoma, depression, AIDS, and wounds.
17. A computer programmed with a homology model of the ligand binding domain of a glucocorticoid receptor according to any of claims 9 to 11.
18. A machine-readable data-storage medium on which has been stored in machine-readable form a homology model of the ligand binding domain of a glucocorticoid receptor according to any of claims 9 to 11.
19. The use of a homology model according to any of claims 9 to 11 as input to a computer programmed for drug design and/or database searching and/or molecular graphic imaging in order to identify new ligands for the glucocorticoid receptor.
20. A computational and chemical method of iteratively generating a homology model of the ligand binding domain of a glucocorticoid receptor, which homology model is capable of being displayed as a three-dimensional image, the method comprising:
- (i) entering into a computer an amino acid sequence and an x-ray crystallographic structure of the ligand binding domain of a thyroid, estrogen or progesterone receptor;
  - (ii) modifying under computer control said x-ray crystallographic structure to take account of known differences between the amino acid configuration of the ligand

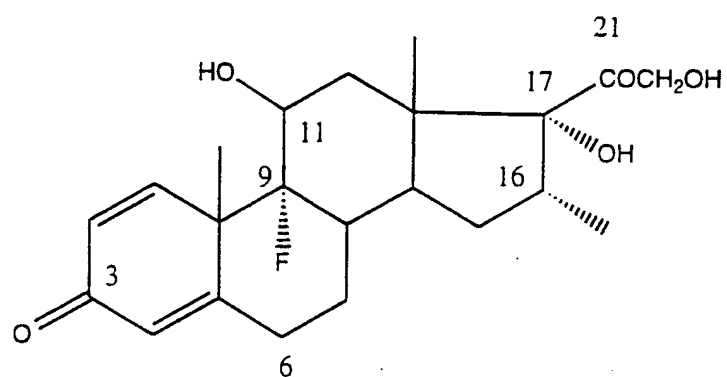
binding domains of the glucocorticoid receptor on the one hand and at least one of the thyroid, estrogen, or progesterone receptors on the other hand,

(iii) reconciling under computer control the resulting modified crystallographic structure with the chemically-determined binding properties of a number of ligands for the glucocorticoid receptor;

(iv) identifying by chemical means the amino acids that line the binding cavity of the ligand binding domain and reconciling under computer control the modified crystallographic structure with these;

(v) repeating steps (ii) and (iii).

Fig. 1



Dexamethasone

2/208

FIGURE 2A

TR_t3cyatocys	RPEPTPEEWDLIHVATEAHRSTNAQGSAAWKORRAFLPDDIGASPIVSMPPDGAVDLEAFS
TRb_triac2	KPEPTDEEWELIKTVTEAHVATNAQGSAAWKQR-KFLPEDIG-----QVDLEAFS
erhum7	----SLALSLTADQMVSALLDAEPPPI-LYSEYDPTRP-----FSE-----ASMMG
grmodel	----PATLPQLTPTLVSLLEVIEPEV-LYAGYDSSVP-----DST-----WRIMT
TR_t3cyatocys	EFTAIITPAITRVVDFAKKLPMAELPCEDQIILLKGCCMEIMSLRAAVRYDPASD--TL
TRb_triac2	HFTAIITPAITRVVDFAKKLPMAELPCEDQIILLKGCCMEIMSLRAAVRYDPASE--TL
erhum7	LLTNLADRELVHMINWAKRVPGFVDLTLDQVHLLCAWLEILMIGLVWRSMHEPG--KL
grmodel	TLNMLGGRQVIAAVKWAKAIPGFRNLHLDQMTLLQYSWMFLMAFALGWSYRQSSANLL
TR_t3cyatocys	TLSGEMAVKREQLKN-GGLGVVSDAIFALGKSLSAFALDDTEVALLQAVLLMST-----D
TRb_triac2	TLNGEMAVTRGQLKN-GGLGVVSDAIFDLGMSLSSFNLDDTEVALLQAVLLMSS-----D
erhum7	LFAPNLLLDRNQKCVEGMVEIFDMLLATSSRFRMMNLQGEFVCLKSIILLNSGVYTF
grmodel	CFAPDLIINEQRMTL-PCMYDQCKHMLYVSSSELHRLQVSYEEYLCMKTLLLLS-----SVP
TR_t3cyatocys	RAGLLCVDAIAASQAAYLLAFEHYVNRK-----HAIPHFWPKLLMKVTDLRMIGACHA
TRb_triac2	RPGLACVERIEKYQDSFLLAFEHYINRK-----HVTWFHPKLLMKVTDLRMIGACHA
erhum7	SSTLKSLEEKDHIHRVLDKITDTLIHLMKAGLTLOQQHQRQAQLLLILSHIRHMSNKG
grmodel	KDGLKSQELFDEIRMTYIKELGKAIVKREGN---SSQNWQRFYQLTKLLDSMHEVVENLL
TR_t3cyatocys	SRFAHMKVECPTA---LFPPPLFLEV
TRb_triac2	SRFLHMKVACPTA---LFPPPLFVAVF
erhum7	EHLYSMKCKN---VVP-LYDLLLEMLDAHR
grmodel	NYCFQTFLD-K-TMSIEFPMLAEIITNQI

3/208

FIGURE 2B

ere_ref4_a	SLALSLTADQMVSALLDAEPPI-LYSEYDPTRP-----FSE-----ASMMGLLTN
lere-kb	SLALSLTADQMVSALLDAEPPI-LYSE-----FSE-----ASMMGLLTN
erhum7	SLALSLTADQMVSALLDAEPPI-LYSEYDPTRP-----FSE-----ASMMGLLTN
grmodelfrer	PATLPQLTPTLVSLLEVIEPEV-LYAGYDSSVP-----DST-----WRIMTTLNM
ere_ref4_a	LADRELVHMINWAKRVPGFVDLTLHDQVHLLCAWLEILMIGLVWRSMHPG--KLLFAP
lere-kb	LADRELVHMINWAKRVPGFVDLTLHDQVHLLCAWLEILMIGLVWRSMHPG--KLLFAP
erhum7	LADRELVHMINWAKRVPGFVDLTLHDQVHLLCAWLEILMIGLVWRSMHPG--KLLFAP
grmodelfrer	LGGRQVIAAVKWAKAIPGFRNLHLDQMTLLOYSWMFLMAFALGWRSYRQSSANLLCFAP
ere_ref4_a	NLLLDNRNQGKCEGMVEIFDMLLATSSRFRMMNLOGEEFVCLKSIILLNSGVYTF---TL
lere-kb	NLLLDNRNQGKCEGMVEIFDMLLATSSRFRMMNLOGEEFVCLKSIILLNSGVYTF---TL
erhum7	NLLLDNRNQGKCEGMVEIFDMLLATSSRFRMMNLOGEEFVCLKSIILLNSGVYTF---TL
grmodelfrer	DLIINEQRM TL-PCMYDQCKHMLYVSSELHRLQVSYEYLCMKITLLLS----SVPKDGL
ere_ref4_a	KSLEEKDHIHRVLDKITDTLIHLMAGLTLQQQHORLAQLLLLILSHIRHMSNKGMEHLY
lere-kb	KSLEEKDHIHRVLDKITDTLIHLMAGLTLQQQHORLAQLLLLILSHIRHMSNKGMEHLY
erhum7	KSLEEKDHIHRVLDKITDTLIHLMAGLTLQQQHORLAQLLLLILSHIRHMSNKGMEHLY
grmodelfrer	KSQELFDEIRMTYIKELGKAIVKREGN---SSQNWORFYQLTKLLDSMHEVVENLLNYCF
ere_ref4_a	SMKCKN---VVP-LYDLLLEMLDAHR
lere-kb	SMKCKN---VVP-LYDLLLEMLDAHR
erhum7	SMKCKN---VVP-LYDLLLEMLDAHR
grmodelfrer	QTF LD-K-TMSIEFPEMLAEITITNQI

4/208

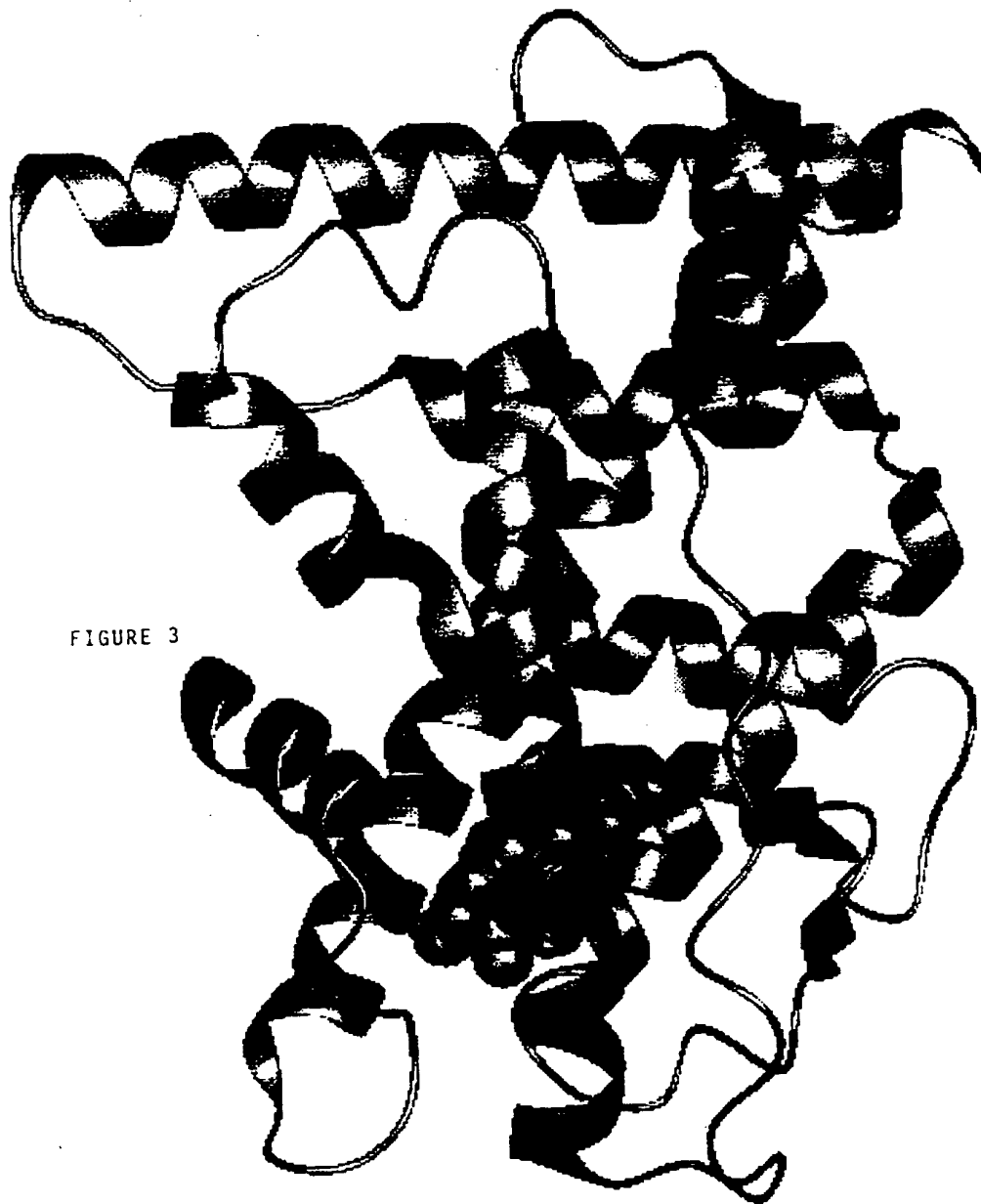
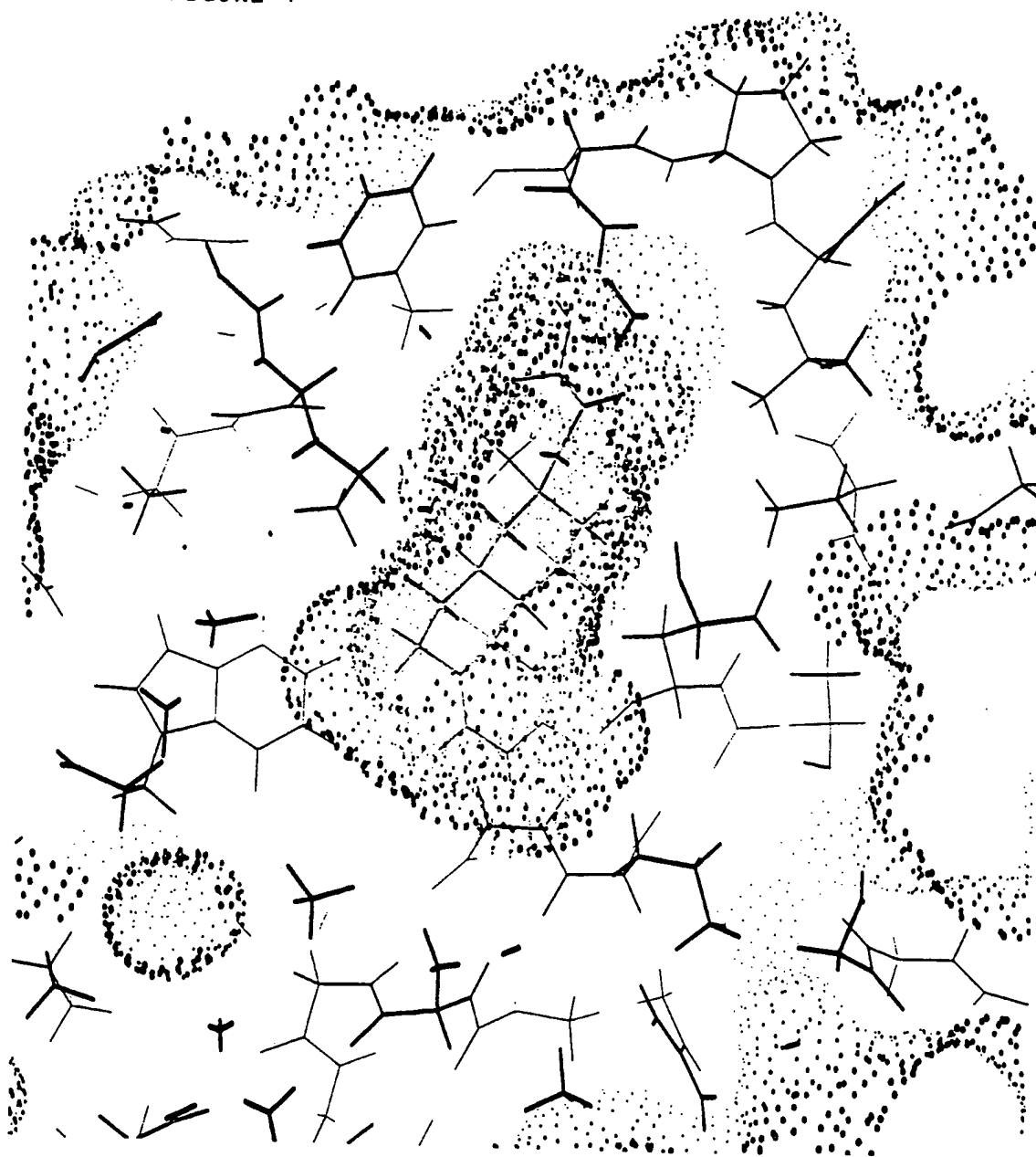
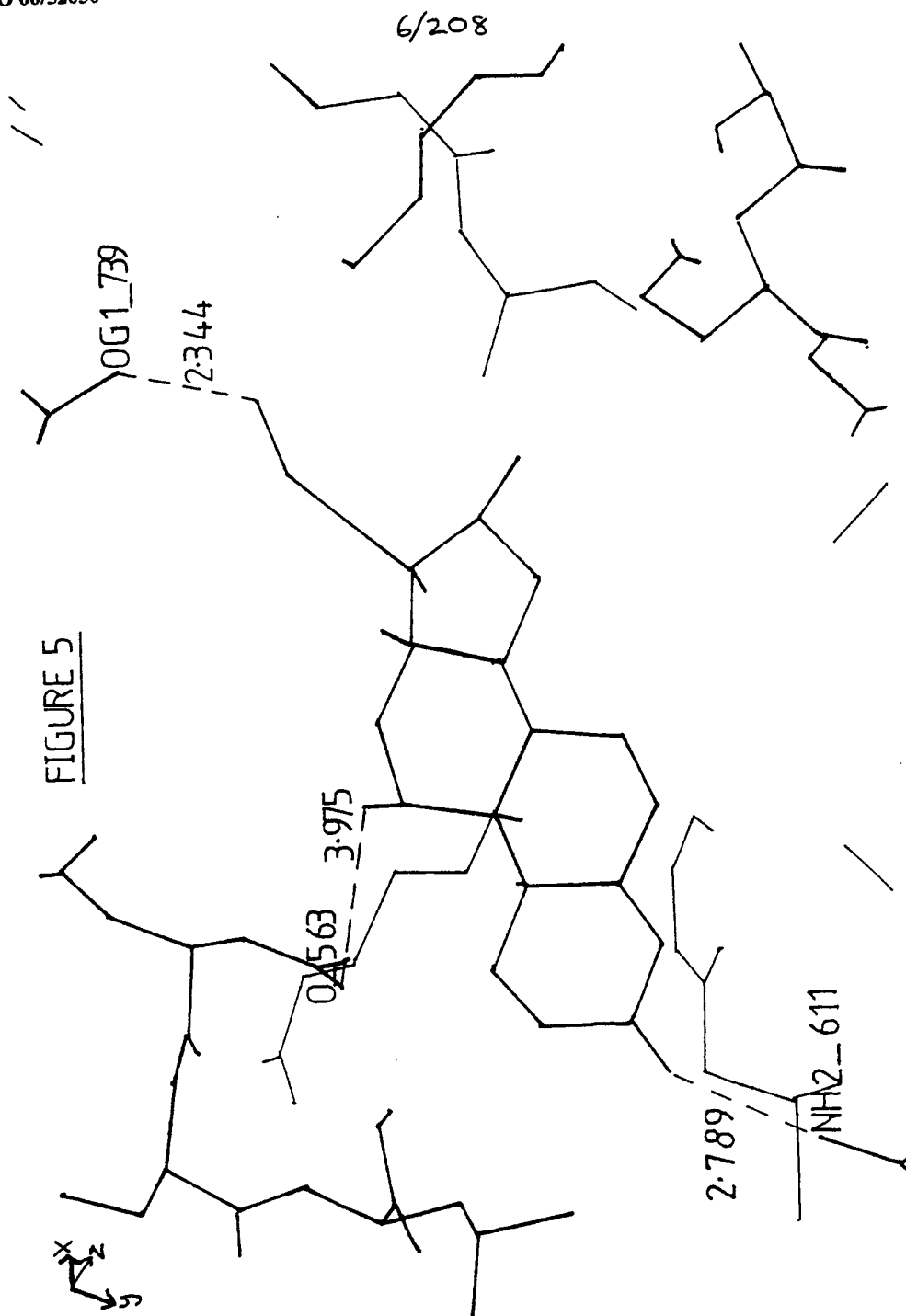


FIGURE 3

5/208

FIGURE 4







7/208

ER 305 SLALSLTADQMVSAALLDAEPPILYSEYDPTTRPFSEASMMGLLTNLADRELVHMINWAKRV  
GR 522 PATLPQLTPTLVSLLEVIEPEVLYAGYDSSVPDSTWRIMTTLNMLGGRQVIAAVKWAKAI

ER 365 PGFVDLTLHDQVHLLLECAWLEILMIGLVWRSMHEPG--KLLFAPNLLLDNRNQGKCVEGMV  
GR 582 PGFRNLHLDDQMTLLQYSWMFLMAFALGWRSYRQSSANLLCFAPDLIINEQRM TL-PCMY

ER 423 EIFDMLLATSSRFRMMNLQGEFVCLKSIIILLNSGVYTFLLSSTLKSLEEKDHIHRVLDKI  
GR 643 DQCKHMLYVSSSELHRLQVSYEEYLCMKTLSSVVPKDG----LKSQELFDEIRMTYIKE

ER 483 TDTLIHLMAKAGLTLOQQHQRLAQLLILSHIRHMSNKGMEHLYSMKCKN--VVP-LYDL  
GR 697 LGKAIVKREGN---SSQNWORFYQLTKLLDSMHEVVENLLNYCFQTFD-KTMSIEFP

ER 540 LLEMLDAHR  
GR 753 LAEIIITNOI

FIG. 6

8/208

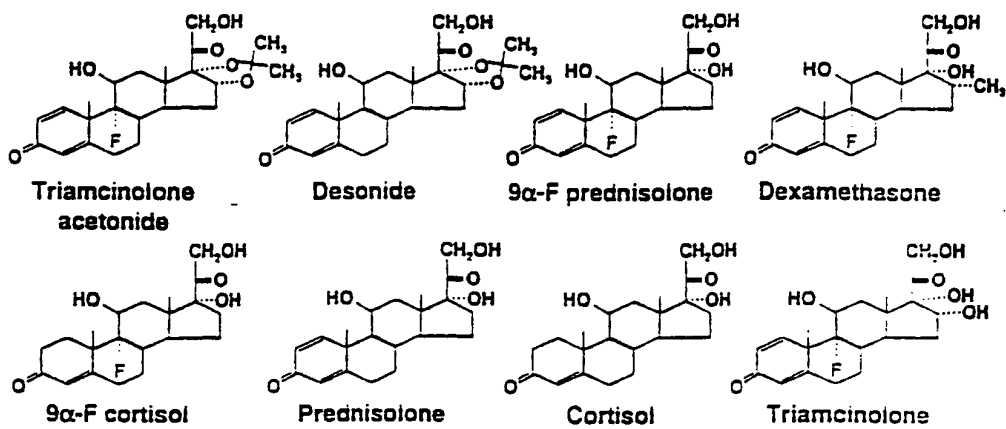


FIG. 7

9/208

Fig 8(i).

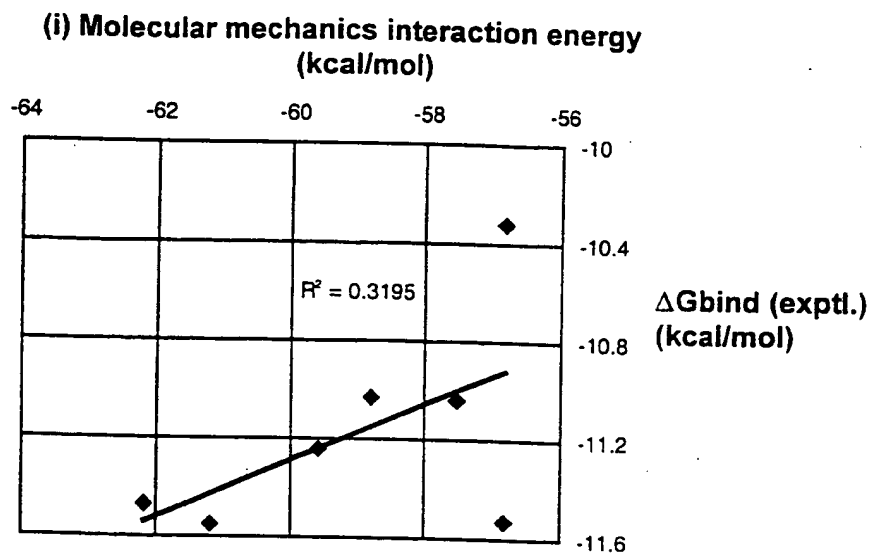
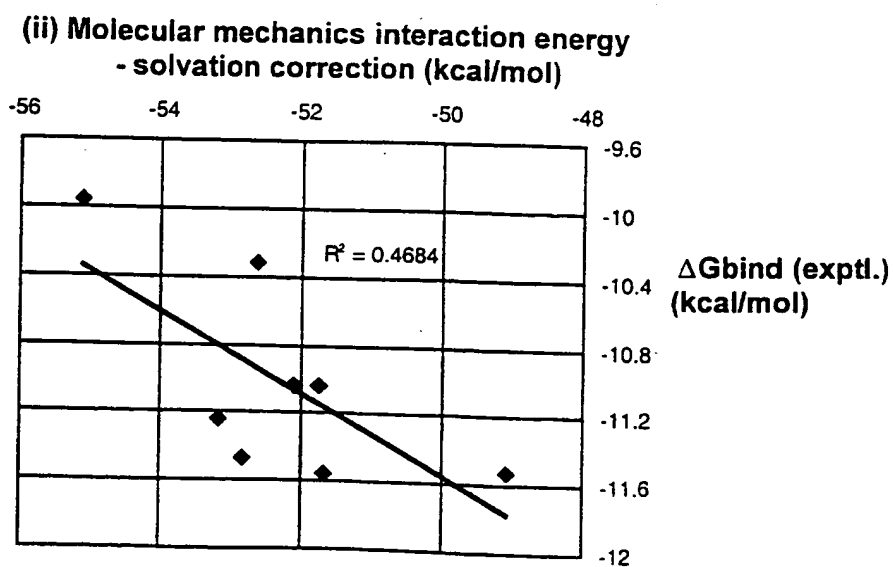


Fig 8(ii).



10/208

Fig 8(iii).

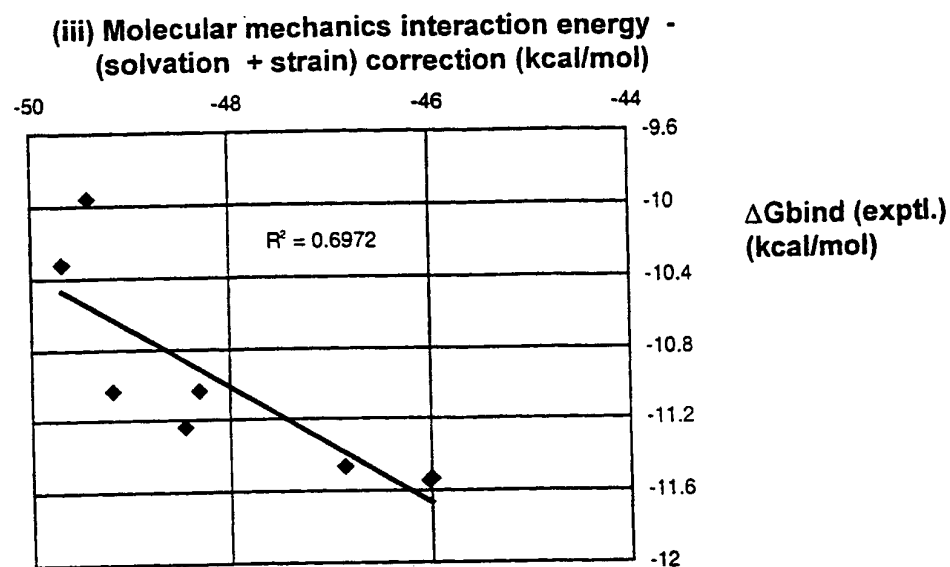
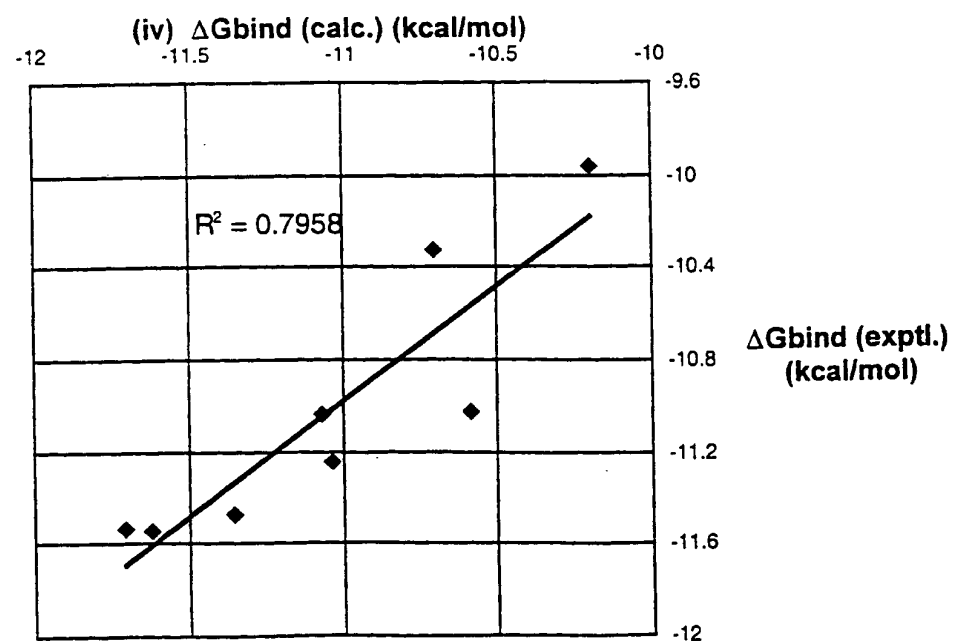


Fig 8(iv).



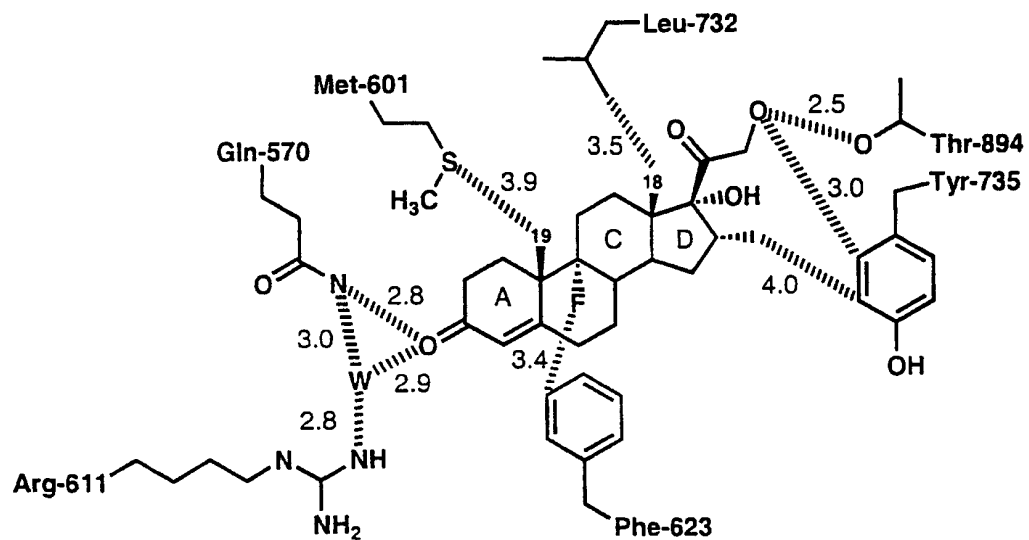
**Figure 9:** (a) RasMol representation of the main interactions with dexamethasone in the GR homology model.  
(b) Sketch of the main interactions with dexamethasone in the GR homology model.

**Figure 9a:**



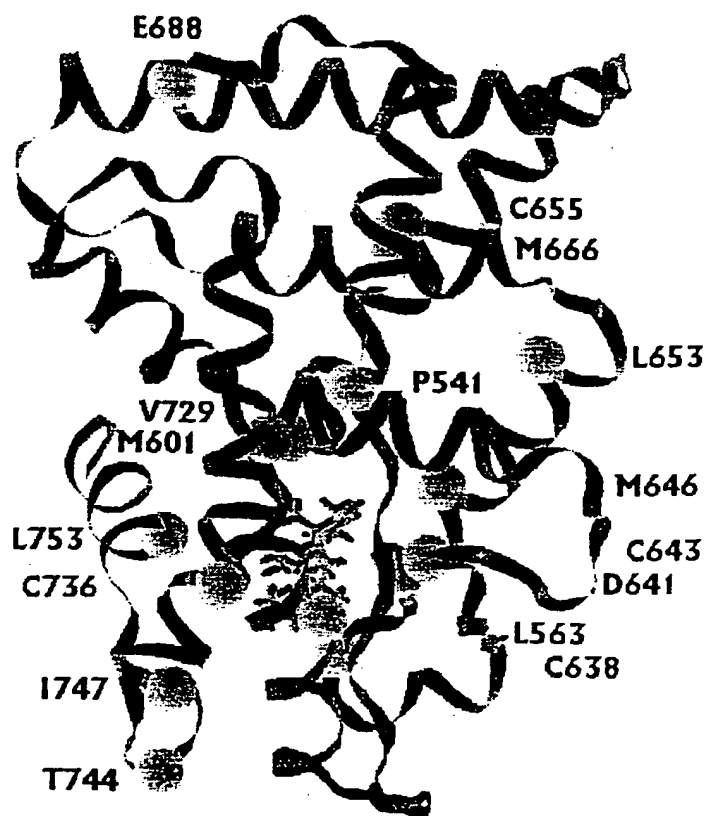
12/208

Figure 9b:



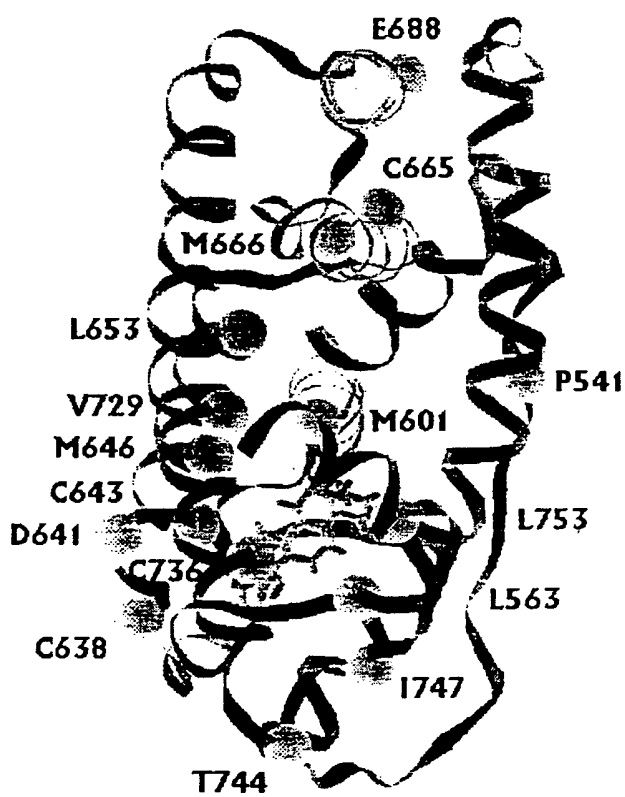
13/208

Figure 10a



14/208

Figure 10b





15/208

progA

QLIPPLINLLMSIEPDVIYAGHDNTKPDTSLLTSLNQLGERQLLSVVKWSKSLPGFRNLHIDDQITLIQYSWM

GRmodel

QLTPTLVSLLEVIEPEVLYAGYDSSVPDSTWRIMTTLNMLGGRQVIAAVKWAKAIPGFRNLHDDQMTLLQYSWM

progA

SLMVFGWGWSYKHVSGQMLYFAPDLILNEQRMKESFYSLCLTMWQIPQEFVKLQVSQEEFLCMKVLLLLNTIP

GRmodel

FLMAFALGWRSYRQSSANLLCFAPDLIINEQRMTPCMYDQCKHMLYVSSELHRLQVSYEEYLCMKTLILLSSVP

progA

LEGLRSQTQFEEMRSSYTRELKAIGLRQKGVVSSQRFYQLTKLLDNLHDLVKQLHLYCLNTFIQSRALSVEFP

GRmodel

KDGLKSQELFDEIRMTYIKELGKAIVKREGNSSQNWQRFYQLTKLLDSMHEVVENLLNYCFQTFDKT-MSIEFP

progA

EMMSEVIAAQLPKILAGMVKPLLCHK\*

GRmodel

EMLAEITNQPKYSNGNIKKLLFHQK\*

Figure 11

16/208

Fig 12

REMARK	1	grfromer						
ATOM	1	C25	CORTC	1	-6.118	0.501	0.557	1.00 0.00
ATOM	2	C26	CORTC	1	-5.161	1.475	0.031	1.00 0.00
ATOM	3	C27	CORTC	1	-4.017	1.077	-0.556	1.00 0.00
ATOM	4	C28	CORTC	1	-3.103	2.102	-1.174	1.00 0.00
ATOM	5	C29	CORTC	1	-1.725	2.081	-0.520	1.00 0.00
ATOM	6	C30	CORTC	1	-1.098	0.688	-0.620	1.00 0.00
ATOM	7	C31	CORTC	1	-2.015	-0.396	-0.015	1.00 0.00
ATOM	8	C32	CORTC	1	-3.481	-0.348	-0.549	1.00 0.00
ATOM	9	C33	CORTC	1	-1.345	-1.804	-0.010	1.00 0.00
ATOM	10	C34	CORTC	1	0.095	-1.803	0.562	1.00 0.00
ATOM	11	C35	CORTC	1	0.975	-0.693	-0.029	1.00 0.00
ATOM	12	C36	CORTC	1	0.223	0.626	0.150	1.00 0.00
ATOM	13	C37	CORTC	1	1.250	1.733	-0.047	1.00 0.00
ATOM	14	C38	CORTC	1	2.589	1.090	0.347	1.00 0.00
ATOM	15	C39	CORTC	1	2.249	-0.345	0.791	1.00 0.00
ATOM	16	C40	CORTC	1	1.281	-0.984	-1.518	1.00 0.00
ATOM	17	C41	CORTC	1	-3.619	-0.828	-2.006	1.00 0.00
ATOM	18	C42	CORTC	1	3.489	-1.254	0.722	1.00 0.00
ATOM	19	C43	CORTC	1	3.976	-1.849	-0.588	1.00 0.00
ATOM	20	O6	CORTC	1	-7.096	0.859	1.135	1.00 0.00
ATOM	21	O7	CORTC	1	-1.342	-2.343	-1.318	1.00 0.00
ATOM	22	O8	CORTC	1	1.923	-0.291	2.164	1.00 0.00
ATOM	23	O9	CORTC	1	4.130	-1.424	1.716	1.00 0.00
ATOM	24	O10	CORTC	1	5.346	-2.133	-0.475	1.00 0.00
ATOM	25	C1	CORTC	1	-4.352	-1.232	0.378	1.00 0.00
ATOM	26	C2	CORTC	1	-5.853	-0.959	0.270	1.00 0.00
ATOM	27	H1	CORTC	1	-5.413	2.513	0.111	1.00 0.00
ATOM	28	2H	CORTC	1	-3.538	3.095	-1.080	1.00 0.00
ATOM	29	3H	CORTC	1	-3.020	1.915	-2.245	1.00 0.00
ATOM	30	4H	CORTC	1	-1.800	2.387	0.522	1.00 0.00
ATOM	31	5H	CORTC	1	-1.082	2.820	-0.997	1.00 0.00
ATOM	32	H6	CORTC	1	-0.941	0.487	-1.676	1.00 0.00
ATOM	33	H7	CORTC	1	-2.102	-0.127	1.040	1.00 0.00
ATOM	34	H8	CORTC	1	-1.953	-2.446	0.630	1.00 0.00
ATOM	35	9H	CORTC	1	0.583	-2.771	0.467	1.00 0.00
ATOM	36	OH1	CORTC	1	0.039	-1.632	1.634	1.00 0.00
ATOM	37	H11	CORTC	1	-0.041	0.700	1.208	1.00 0.00
ATOM	38	2H1	CORTC	1	1.001	2.576	0.593	1.00 0.00
ATOM	39	3H1	CORTC	1	1.263	2.094	-1.070	1.00 0.00
ATOM	40	4H1	CORTC	1	3.089	1.642	1.136	1.00 0.00
ATOM	41	5H1	CORTC	1	3.255	1.090	-0.518	1.00 0.00
ATOM	42	6H1	CORTC	1	1.927	-0.232	-1.968	1.00 0.00
ATOM	43	7H1	CORTC	1	0.373	-1.012	-2.114	1.00 0.00
ATOM	44	8H1	CORTC	1	1.701	-1.973	-1.671	1.00 0.00
ATOM	45	9H1	CORTC	1	-3.452	-1.901	-2.089	1.00 0.00
ATOM	46	OH2	CORTC	1	-2.887	-0.350	-2.656	1.00 0.00
ATOM	47	1H2	CORTC	1	-4.607	-0.626	-2.414	1.00 0.00
ATOM	48	2H2	CORTC	1	3.848	-1.145	-1.410	1.00 0.00

17/208

ATOM	49	3H2	CORTC	1	3.440	-2.777	-0.796	1.00	0.00
ATOM	50	H24	CORTC	1	-1.053	-3.251	-1.314	1.00	0.00
ATOM	51	H25	CORTC	1	2.683	-0.664	2.614	1.00	0.00
ATOM	52	H26	CORTC	1	5.547	-2.208	0.462	1.00	0.00
ATOM	53	7H2	CORTC	1	-4.156	-2.281	0.172	1.00	0.00
ATOM	54	8H2	CORTC	1	-4.062	-1.081	1.420	1.00	0.00
ATOM	55	9H2	CORTC	1	-6.416	-1.567	0.975	1.00	0.00
ATOM	56	0H3	CORTC	1	-6.218	-1.167	-0.729	1.00	0.00
ATOM	57	N	ALA A 523		-25.079	3.809	-23.074	1.00	0.00
ATOM	58	CA	ALA A 523		-25.892	4.487	-22.104	1.00	0.00
ATOM	59	C	ALA A 523		-25.170	5.680	-21.569	1.00	0.00
ATOM	60	O	ALA A 523		-25.779	6.716	-21.305	1.00	0.00
ATOM	61	CB	ALA A 523		-26.253	3.589	-20.908	1.00	0.00
ATOM	62	1HT	ALA A 523		-24.576	4.510	-23.655	1.00	0.00
ATOM	63	2HT	ALA A 523		-25.684	3.224	-23.685	1.00	0.00
ATOM	64	HA	ALA A 523		-26.802	4.813	-22.608	1.00	0.00
ATOM	65	1HB	ALA A 523		-25.353	3.249	-20.396	1.00	0.00
ATOM	66	2HB	ALA A 523		-26.799	2.709	-21.249	1.00	0.00
ATOM	67	3HB	ALA A 523		-26.860	4.142	-20.192	1.00	0.00
ATOM	68	N	THR A 524		-23.837	5.574	-21.425	1.00	0.00
ATOM	69	CA	THR A 524		-23.081	6.641	-20.839	1.00	0.00
ATOM	70	C	THR A 524		-23.327	7.904	-21.606	1.00	0.00
ATOM	71	O	THR A 524		-23.479	8.972	-21.015	1.00	0.00
ATOM	72	CB	THR A 524		-21.605	6.372	-20.834	1.00	0.00
ATOM	73	OG1	THR A 524		-20.927	7.391	-20.114	1.00	0.00
ATOM	74	CG2	THR A 524		-21.100	6.307	-22.283	1.00	0.00
ATOM	75	HN	THR A 524		-23.370	4.744	-21.729	1.00	0.00
ATOM	76	HA	THR A 524		-23.444	6.758	-19.818	1.00	0.00
ATOM	77	HB	THR A 524		-21.396	5.417	-20.352	1.00	0.00
ATOM	78	HG1	THR A 524		-20.005	7.175	-20.141	1.00	0.00
ATOM	79	1HG2	THR A 524		-20.958	7.310	-22.687	1.00	0.00
ATOM	80	2HG2	THR A 524		-21.825	5.791	-22.912	1.00	0.00
ATOM	81	3HG2	THR A 524		-20.142	5.788	-22.325	1.00	0.00
ATOM	82	N	LEU A 525		-23.397	7.817	-22.944	1.00	0.00
ATOM	83	CA	LEU A 525		-23.570	8.996	-23.745	1.00	0.00
ATOM	84	C	LEU A 525		-24.870	9.732	-23.529	1.00	0.00
ATOM	85	O	LEU A 525		-24.865	10.960	-23.499	1.00	0.00
ATOM	86	CB	LEU A 525		-23.420	8.705	-25.245	1.00	0.00
ATOM	87	CG	LEU A 525		-21.995	8.237	-25.583	1.00	0.00
ATOM	88	CD1	LEU A 525		-21.773	8.118	-27.099	1.00	0.00
ATOM	89	CD2	LEU A 525		-20.953	9.122	-24.879	1.00	0.00
ATOM	90	HN	LEU A 525		-23.329	6.923	-23.385	1.00	0.00
ATOM	91	HA	LEU A 525		-22.812	9.710	-23.422	1.00	0.00
ATOM	92	1HB	LEU A 525		-23.647	9.608	-25.812	1.00	0.00
ATOM	93	2HB	LEU A 525		-24.132	7.932	-25.535	1.00	0.00
ATOM	94	HG	LEU A 525		-21.818	7.266	-25.119	1.00	0.00
ATOM	95	1HD1	LEU A 525		-21.928	9.081	-27.587	1.00	0.00
ATOM	96	2HD1	LEU A 525		-22.478	7.406	-27.528	1.00	0.00
ATOM	97	3HD1	LEU A 525		-20.753	7.795	-27.307	1.00	0.00

18/208

ATOM	98	1HD2 LEU A 525	-21.080	9.079	-23.798	1.00	0.00
ATOM	99	2HD2 LEU A 525	-21.069	10.159	-25.192	1.00	0.00
ATOM	100	3HD2 LEU A 525	-19.946	8.778	-25.115	1.00	0.00
ATOM	101	N PRO A 526	-25.994	9.073	-23.434	1.00	0.00
ATOM	102	CA PRO A 526	-27.215	9.811	-23.205	1.00	0.00
ATOM	103	C PRO A 526	-27.475	10.277	-21.807	1.00	0.00
ATOM	104	O PRO A 526	-28.343	11.129	-21.629	1.00	0.00
ATOM	105	CB PRO A 526	-28.359	8.964	-23.770	1.00	0.00
ATOM	106	CG PRO A 526	-27.711	7.626	-24.150	1.00	0.00
ATOM	107	CD PRO A 526	-26.240	7.996	-24.368	1.00	0.00
ATOM	108	1HD PRO A 526	-25.584	7.152	-24.155	1.00	0.00
ATOM	109	2HD PRO A 526	-26.063	8.330	-25.390	1.00	0.00
ATOM	110	HA PRO A 526	-27.163	10.776	-23.710	1.00	0.00
ATOM	111	1HB PRO A 526	-28.804	9.443	-24.642	1.00	0.00
ATOM	112	2HB PRO A 526	-29.142	8.821	-23.024	1.00	0.00
ATOM	113	1HG PRO A 526	-27.821	6.892	-23.352	1.00	0.00
ATOM	114	2HG PRO A 526	-28.155	7.214	-25.056	1.00	0.00
ATOM	115	N GLN A 527	-26.761	9.739	-20.807	1.00	0.00
ATOM	116	CA GLN A 527	-26.993	10.096	-19.439	1.00	0.00
ATOM	117	C GLN A 527	-26.834	11.582	-19.328	1.00	0.00
ATOM	118	O GLN A 527	-26.010	12.175	-20.021	1.00	0.00
ATOM	119	CB GLN A 527	-25.919	9.467	-18.537	1.00	0.00
ATOM	120	CG GLN A 527	-26.244	9.400	-17.051	1.00	0.00
ATOM	121	CD GLN A 527	-26.605	7.951	-16.765	1.00	0.00
ATOM	122	OE1 GLN A 527	-27.358	7.323	-17.507	1.00	0.00
ATOM	123	NE2 GLN A 527	-26.039	7.397	-15.658	1.00	0.00
ATOM	124	HN GLN A 527	-26.049	9.072	-21.023	1.00	0.00
ATOM	125	HA GLN A 527	-27.984	9.731	-19.171	1.00	0.00
ATOM	126	1HB GLN A 527	-25.002	10.042	-18.655	1.00	0.00
ATOM	127	2HB GLN A 527	-25.737	8.453	-18.888	1.00	0.00
ATOM	128	1HG GLN A 527	-27.087	10.046	-16.805	1.00	0.00
ATOM	129	2HG GLN A 527	-25.384	9.692	-16.449	1.00	0.00
ATOM	130	1HE2 GLN A 527	-25.549	7.978	-15.009	1.00	0.00
ATOM	131	2HE2 GLN A 527	-26.104	6.416	-15.480	1.00	0.00
ATOM	132	N LEU A 528	-27.646	12.238	-18.474	1.00	0.00
ATOM	133	CA LEU A 528	-27.439	13.647	-18.292	1.00	0.00
ATOM	134	C LEU A 528	-26.548	13.763	-17.108	1.00	0.00
ATOM	135	O LEU A 528	-26.401	12.807	-16.350	1.00	0.00
ATOM	136	CB LEU A 528	-28.701	14.500	-18.039	1.00	0.00
ATOM	137	CG LEU A 528	-29.630	14.017	-16.911	1.00	0.00
ATOM	138	CD1 LEU A 528	-30.808	14.986	-16.720	1.00	0.00
ATOM	139	CD2 LEU A 528	-30.129	12.591	-17.179	1.00	0.00
ATOM	140	HN LEU A 528	-28.370	11.756	-17.981	1.00	0.00
ATOM	141	HA LEU A 528	-26.948	13.992	-19.201	1.00	0.00
ATOM	142	1HB LEU A 528	-29.278	14.529	-18.962	1.00	0.00
ATOM	143	2HB LEU A 528	-28.381	15.512	-17.802	1.00	0.00
ATOM	144	HG LEU A 528	-29.065	13.946	-15.982	1.00	0.00
ATOM	145	1HD1 LEU A 528	-31.397	15.063	-17.634	1.00	0.00
ATOM	146	2HD1 LEU A 528	-30.440	15.981	-16.471	1.00	0.00

19/208

ATOM	147	3HD1	LEU A 528	-31.464	14.629	-15.926	1.00	0.00
ATOM	148	1HD2	LEU A 528	-29.370	11.859	-16.903	1.00	0.00
ATOM	149	2HD2	LEU A 528	-30.352	12.463	-18.238	1.00	0.00
ATOM	150	3HD2	LEU A 528	-31.023	12.388	-16.590	1.00	0.00
ATOM	151	N	THR A 529	-25.953	14.955	-16.901	1.00	0.00
ATOM	152	CA	THR A 529	-25.011	15.088	-15.833	1.00	0.00
ATOM	153	C	THR A 529	-25.630	14.696	-14.530	1.00	0.00
ATOM	154	O	THR A 529	-24.911	14.143	-13.703	1.00	0.00
ATOM	155	CB	THR A 529	-24.318	16.430	-15.759	1.00	0.00
ATOM	156	OG1	THR A 529	-23.408	16.443	-14.668	1.00	0.00
ATOM	157	CG2	THR A 529	-25.318	17.588	-15.674	1.00	0.00
ATOM	158	HN	THR A 529	-26.168	15.736	-17.487	1.00	0.00
ATOM	159	HA	THR A 529	-24.272	14.301	-15.982	1.00	0.00
ATOM	160	HB	THR A 529	-23.757	16.618	-16.675	1.00	0.00
ATOM	161	HG1	THR A 529	-23.922	16.603	-13.887	1.00	0.00
ATOM	162	1HG2	THR A 529	-25.690	17.702	-14.656	1.00	0.00
ATOM	163	2HG2	THR A 529	-26.171	17.398	-16.325	1.00	0.00
ATOM	164	3HG2	THR A 529	-24.837	18.523	-15.963	1.00	0.00
ATOM	165	N	PRO A 530	-26.897	14.913	-14.259	1.00	0.00
ATOM	166	CA	PRO A 530	-27.417	14.458	-13.003	1.00	0.00
ATOM	167	C	PRO A 530	-27.432	12.964	-12.906	1.00	0.00
ATOM	168	O	PRO A 530	-27.159	12.442	-11.828	1.00	0.00
ATOM	169	CB	PRO A 530	-28.805	15.078	-12.859	1.00	0.00
ATOM	170	CG	PRO A 530	-28.734	16.338	-13.737	1.00	0.00
ATOM	171	CD	PRO A 530	-27.709	15.980	-14.825	1.00	0.00
ATOM	172	1HD	PRO A 530	-28.205	15.633	-15.732	1.00	0.00
ATOM	173	2HD	PRO A 530	-27.083	16.837	-15.072	1.00	0.00
ATOM	174	HA	PRO A 530	-26.763	14.779	-12.192	1.00	0.00
ATOM	175	1HB	PRO A 530	-29.018	15.333	-11.820	1.00	0.00
ATOM	176	2HB	PRO A 530	-29.580	14.397	-13.208	1.00	0.00
ATOM	177	1HG	PRO A 530	-29.706	16.569	-14.173	1.00	0.00
ATOM	178	2HG	PRO A 530	-28.407	17.203	-13.159	1.00	0.00
ATOM	179	N	THR A 531	-27.761	12.252	-14.004	1.00	0.00
ATOM	180	CA	THR A 531	-27.830	10.823	-13.907	1.00	0.00
ATOM	181	C	THR A 531	-26.461	10.248	-13.760	1.00	0.00
ATOM	182	O	THR A 531	-26.269	9.282	-13.024	1.00	0.00
ATOM	183	CB	THR A 531	-28.499	10.141	-15.059	1.00	0.00
ATOM	184	OG1	THR A 531	-29.816	10.643	-15.223	1.00	0.00
ATOM	185	CG2	THR A 531	-28.587	8.645	-14.709	1.00	0.00
ATOM	186	HN	THR A 531	-27.953	12.714	-14.870	1.00	0.00
ATOM	187	HA	THR A 531	-28.377	10.609	-12.989	1.00	0.00
ATOM	188	HB	THR A 531	-27.947	10.324	-15.981	1.00	0.00
ATOM	189	HG1	THR A 531	-30.229	10.607	-14.371	1.00	0.00
ATOM	190	1HG2	THR A 531	-29.305	8.479	-13.906	1.00	0.00
ATOM	191	2HG2	THR A 531	-27.616	8.280	-14.373	1.00	0.00
ATOM	192	3HG2	THR A 531	-28.913	8.073	-15.577	1.00	0.00
ATOM	193	N	LEU A 532	-25.463	10.834	-14.449	1.00	0.00
ATOM	194	CA	LEU A 532	-24.140	10.293	-14.341	1.00	0.00
ATOM	195	C	LEU A 532	-23.728	10.336	-12.904	1.00	0.00

20/208

ATOM	196	O	LEU A 532	-23.216	9.356	-12.375	1.00	0.00
ATOM	197	CB	LEU A 532	-23.037	11.072	-15.092	1.00	0.00
ATOM	198	CG	LEU A 532	-22.979	10.907	-16.625	1.00	0.00
ATOM	199	CD1	LEU A 532	-24.194	11.521	-17.322	1.00	0.00
ATOM	200	CD2	LEU A 532	-21.656	11.457	-17.184	1.00	0.00
ATOM	201	HN	LEU A 532	-25.643	11.632	-15.025	1.00	0.00
ATOM	202	HA	LEU A 532	-24.200	9.278	-14.735	1.00	0.00
ATOM	203	1HB	LEU A 532	-22.076	10.760	-14.688	1.00	0.00
ATOM	204	2HB	LEU A 532	-23.173	12.130	-14.877	1.00	0.00
ATOM	205	HG	LEU A 532	-22.929	9.846	-16.866	1.00	0.00
ATOM	206	1HD1	LEU A 532	-24.165	12.609	-17.261	1.00	0.00
ATOM	207	2HD1	LEU A 532	-25.113	11.182	-16.844	1.00	0.00
ATOM	208	3HD1	LEU A 532	-24.204	11.243	-18.376	1.00	0.00
ATOM	209	1HD2	LEU A 532	-20.824	11.200	-16.528	1.00	0.00
ATOM	210	2HD2	LEU A 532	-21.702	12.543	-17.261	1.00	0.00
ATOM	211	3HD2	LEU A 532	-21.455	11.028	-18.166	1.00	0.00
ATOM	212	N	VAL A 533	-23.988	11.475	-12.229	1.00	0.00
ATOM	213	CA	VAL A 533	-23.557	11.670	-10.872	1.00	0.00
ATOM	214	C	VAL A 533	-24.106	10.569	-10.040	1.00	0.00
ATOM	215	O	VAL A 533	-23.395	9.938	-9.260	1.00	0.00
ATOM	216	CB	VAL A 533	-24.181	12.876	-10.230	1.00	0.00
ATOM	217	CG1	VAL A 533	-23.646	13.000	-8.794	1.00	0.00
ATOM	218	CG2	VAL A 533	-23.999	14.111	-11.119	1.00	0.00
ATOM	219	HN	VAL A 533	-24.495	12.205	-12.688	1.00	0.00
ATOM	220	HA	VAL A 533	-22.473	11.779	-10.901	1.00	0.00
ATOM	221	HB	VAL A 533	-25.266	12.772	-10.216	1.00	0.00
ATOM	222	1HG1	VAL A 533	-22.558	12.936	-8.781	1.00	0.00
ATOM	223	2HG1	VAL A 533	-24.039	12.193	-8.175	1.00	0.00
ATOM	224	3HG1	VAL A 533	-23.932	13.961	-8.368	1.00	0.00
ATOM	225	1HG2	VAL A 533	-24.952	14.421	-11.548	1.00	0.00
ATOM	226	2HG2	VAL A 533	-23.317	13.886	-11.940	1.00	0.00
ATOM	227	3HG2	VAL A 533	-23.606	14.942	-10.533	1.00	0.00
ATOM	228	N	SER A 534	-25.416	10.334	-10.198	1.00	0.00
ATOM	229	CA	SER A 534	-26.127	9.359	-9.430	1.00	0.00
ATOM	230	C	SER A 534	-25.601	8.002	-9.723	1.00	0.00
ATOM	231	O	SER A 534	-25.351	7.212	-8.813	1.00	0.00
ATOM	232	CB	SER A 534	-27.617	9.334	-9.788	1.00	0.00
ATOM	233	OG	SER A 534	-28.224	8.203	-9.192	1.00	0.00
ATOM	234	HN	SER A 534	-25.918	10.863	-10.882	1.00	0.00
ATOM	235	HA	SER A 534	-25.993	9.621	-8.381	1.00	0.00
ATOM	236	1HB	SER A 534	-27.748	9.267	-10.868	1.00	0.00
ATOM	237	2HB	SER A 534	-28.113	10.229	-9.415	1.00	0.00
ATOM	238	HG	SER A 534	-27.556	7.532	-9.137	1.00	0.00
ATOM	239	N	LEU A 535	-25.397	7.716	-11.018	1.00	0.00
ATOM	240	CA	LEU A 535	-24.957	6.413	-11.399	1.00	0.00
ATOM	241	C	LEU A 535	-23.671	6.165	-10.706	1.00	0.00
ATOM	242	O	LEU A 535	-23.473	5.109	-10.102	1.00	0.00
ATOM	243	CB	LEU A 535	-24.674	6.303	-12.907	1.00	0.00
ATOM	244	CG	LEU A 535	-24.196	4.904	-13.334	1.00	0.00

21/208

ATOM	245	CD1 LEU A 535	-25.299	3.852	-13.143	1.00	0.00
ATOM	246	CD2 LEU A 535	-23.613	4.922	-14.757	1.00	0.00
ATOM	247	HN LEU A 535	-25.552	8.416	-11.715	1.00	0.00
ATOM	248	HA LEU A 535	-25.748	5.719	-11.114	1.00	0.00
ATOM	249	1HB LEU A 535	-23.909	7.031	-13.174	1.00	0.00
ATOM	250	2HB LEU A 535	-25.584	6.545	-13.454	1.00	0.00
ATOM	251	HG LEU A 535	-23.326	4.625	-12.741	1.00	0.00
ATOM	252	1HD1 LEU A 535	-26.177	4.101	-13.739	1.00	0.00
ATOM	253	2HD1 LEU A 535	-25.602	3.810	-12.097	1.00	0.00
ATOM	254	3HD1 LEU A 535	-24.943	2.872	-13.461	1.00	0.00
ATOM	255	1HD2 LEU A 535	-23.017	5.821	-14.917	1.00	0.00
ATOM	256	2HD2 LEU A 535	-24.416	4.915	-15.493	1.00	0.00
ATOM	257	3HD2 LEU A 535	-22.967	4.058	-14.910	1.00	0.00
ATOM	258	N LEU A 536	-22.765	7.147	-10.741	1.00	0.00
ATOM	259	CA LEU A 536	-21.475	6.943	-10.168	1.00	0.00
ATOM	260	C LEU A 536	-21.618	6.859	-8.676	1.00	0.00
ATOM	261	O LEU A 536	-20.951	6.066	-8.012	1.00	0.00
ATOM	262	CB LEU A 536	-20.499	8.054	-10.577	1.00	0.00
ATOM	263	CG LEU A 536	-19.042	7.574	-10.561	1.00	0.00
ATOM	264	CD1 LEU A 536	-18.532	7.270	-9.152	1.00	0.00
ATOM	265	CD2 LEU A 536	-18.892	6.367	-11.503	1.00	0.00
ATOM	266	HN LEU A 536	-22.991	8.022	-11.168	1.00	0.00
ATOM	267	HA LEU A 536	-21.118	5.975	-10.521	1.00	0.00
ATOM	268	1HB LEU A 536	-20.606	8.893	-9.889	1.00	0.00
ATOM	269	2HB LEU A 536	-20.751	8.399	-11.579	1.00	0.00
ATOM	270	HG LEU A 536	-18.412	8.343	-11.006	1.00	0.00
ATOM	271	1HD1 LEU A 536	-18.391	6.197	-9.016	1.00	0.00
ATOM	272	2HD1 LEU A 536	-19.253	7.612	-8.409	1.00	0.00
ATOM	273	3HD1 LEU A 536	-17.573	7.760	-8.985	1.00	0.00
ATOM	274	1HD2 LEU A 536	-19.327	6.584	-12.479	1.00	0.00
ATOM	275	2HD2 LEU A 536	-19.408	5.501	-11.089	1.00	0.00
ATOM	276	3HD2 LEU A 536	-17.838	6.132	-11.648	1.00	0.00
ATOM	277	N GLU A 537	-22.536	7.666	-8.113	1.00	0.00
ATOM	278	CA GLU A 537	-22.768	7.706	-6.696	1.00	0.00
ATOM	279	C GLU A 537	-23.166	6.342	-6.225	1.00	0.00
ATOM	280	O GLU A 537	-22.698	5.872	-5.189	1.00	0.00
ATOM	281	CB GLU A 537	-23.943	8.637	-6.345	1.00	0.00
ATOM	282	CG GLU A 537	-24.259	8.742	-4.852	1.00	0.00
ATOM	283	CD GLU A 537	-23.474	9.909	-4.274	1.00	0.00
ATOM	284	OE1 GLU A 537	-23.662	10.204	-3.064	1.00	0.00
ATOM	285	OE2 GLU A 537	-22.684	10.526	-5.036	1.00	0.00
ATOM	286	HN GLU A 537	-23.079	8.261	-8.706	1.00	0.00
ATOM	287	HA GLU A 537	-21.848	8.061	-6.233	1.00	0.00
ATOM	288	1HB GLU A 537	-24.832	8.274	-6.858	1.00	0.00
ATOM	289	2HB GLU A 537	-23.713	9.633	-6.717	1.00	0.00
ATOM	290	1HG GLU A 537	-23.970	7.826	-4.336	1.00	0.00
ATOM	291	2HG GLU A 537	-25.324	8.916	-4.699	1.00	0.00
ATOM	292	N VAL A 538	-24.056	5.672	-6.979	1.00	0.00
ATOM	293	CA VAL A 538	-24.556	4.390	-6.568	1.00	0.00

22/208

ATOM	294	C	VAL A 538	-23.516	3.314	-6.628	1.00	0.00
ATOM	295	O	VAL A 538	-23.511	2.405	-5.803	1.00	0.00
ATOM	296	CB	VAL A 538	-25.740	3.907	-7.362	1.00	0.00
ATOM	297	CG1	VAL A 538	-26.863	4.951	-7.249	1.00	0.00
ATOM	298	CG2	VAL A 538	-25.309	3.563	-8.796	1.00	0.00
ATOM	299	HN	VAL A 538	-24.374	6.073	-7.838	1.00	0.00
ATOM	300	HA	VAL A 538	-24.831	4.491	-5.519	1.00	0.00
ATOM	301	HB	VAL A 538	-26.082	2.947	-6.975	1.00	0.00
ATOM	302	1HG1	VAL A 538	-26.456	5.961	-7.298	1.00	0.00
ATOM	303	2HG1	VAL A 538	-27.383	4.843	-6.297	1.00	0.00
ATOM	304	3HG1	VAL A 538	-27.571	4.833	-8.069	1.00	0.00
ATOM	305	1HG2	VAL A 538	-24.340	3.064	-8.798	1.00	0.00
ATOM	306	2HG2	VAL A 538	-25.221	4.472	-9.391	1.00	0.00
ATOM	307	3HG2	VAL A 538	-26.035	2.893	-9.256	1.00	0.00
ATOM	308	N	ILE A 539	-22.595	3.403	-7.604	1.00	0.00
ATOM	309	CA	ILE A 539	-21.645	2.358	-7.858	1.00	0.00
ATOM	310	C	ILE A 539	-20.761	2.121	-6.681	1.00	0.00
ATOM	311	O	ILE A 539	-20.295	1.000	-6.483	1.00	0.00
ATOM	312	CB	ILE A 539	-20.732	2.669	-8.999	1.00	0.00
ATOM	313	CG1	ILE A 539	-21.553	3.171	-10.195	1.00	0.00
ATOM	314	CG2	ILE A 539	-19.883	1.418	-9.276	1.00	0.00
ATOM	315	CD1	ILE A 539	-22.880	2.440	-10.388	1.00	0.00
ATOM	316	HN	ILE A 539	-22.572	4.225	-8.171	1.00	0.00
ATOM	317	HA	ILE A 539	-22.221	1.458	-8.073	1.00	0.00
ATOM	318	HB	ILE A 539	-20.088	3.512	-8.747	1.00	0.00
ATOM	319	1HG2	ILE A 539	-20.519	0.571	-9.534	1.00	0.00
ATOM	320	2HG2	ILE A 539	-19.307	1.150	-8.391	1.00	0.00
ATOM	321	3HG2	ILE A 539	-19.207	1.600	-10.112	1.00	0.00
ATOM	322	1HG1	ILE A 539	-20.957	3.053	-11.099	1.00	0.00
ATOM	323	2HG1	ILE A 539	-21.757	4.231	-10.055	1.00	0.00
ATOM	324	1HD1	ILE A 539	-23.096	1.801	-9.532	1.00	0.00
ATOM	325	2HD1	ILE A 539	-22.838	1.811	-11.276	1.00	0.00
ATOM	326	3HD1	ILE A 539	-23.694	3.158	-10.486	1.00	0.00
ATOM	327	N	GLU A 540	-20.503	3.188	-5.897	1.00	0.00
ATOM	328	CA	GLU A 540	-19.615	3.196	-4.766	1.00	0.00
ATOM	329	C	GLU A 540	-19.648	1.908	-3.999	1.00	0.00
ATOM	330	O	GLU A 540	-20.702	1.356	-3.687	1.00	0.00
ATOM	331	CB	GLU A 540	-19.933	4.348	-3.798	1.00	0.00
ATOM	332	CG	GLU A 540	-18.850	4.602	-2.757	1.00	0.00
ATOM	333	CD	GLU A 540	-17.667	5.258	-3.455	1.00	0.00
ATOM	334	OE1	GLU A 540	-16.780	5.783	-2.731	1.00	0.00
ATOM	335	OE2	GLU A 540	-17.633	5.248	-4.715	1.00	0.00
ATOM	336	HN	GLU A 540	-20.968	4.044	-6.122	1.00	0.00
ATOM	337	HA	GLU A 540	-18.603	3.298	-5.158	1.00	0.00
ATOM	338	1HB	GLU A 540	-20.864	4.119	-3.282	1.00	0.00
ATOM	339	2HB	GLU A 540	-20.076	5.258	-4.378	1.00	0.00
ATOM	340	1HG	GLU A 540	-18.526	3.664	-2.305	1.00	0.00
ATOM	341	2HG	GLU A 540	-19.219	5.265	-1.975	1.00	0.00
ATOM	342	N	PRO A 541	-18.462	1.416	-3.745	1.00	0.00



23/208

ATOM	343	CA	PRO A 541	-18.293	0.176	-3.033	1.00	0.00
ATOM	344	C	PRO A 541	-18.481	0.367	-1.567	1.00	0.00
ATOM	345	O	PRO A 541	-18.484	1.503	-1.097	1.00	0.00
ATOM	346	CB	PRO A 541	-16.882	-0.311	-3.354	1.00	0.00
ATOM	347	CG	PRO A 541	-16.552	0.357	-4.695	1.00	0.00
ATOM	348	CD	PRO A 541	-17.375	1.652	-4.680	1.00	0.00
ATOM	349	IHD	PRO A 541	-16.771	2.496	-4.348	1.00	0.00
ATOM	350	2HD	PRO A 541	-17.774	1.874	-5.670	1.00	0.00
ATOM	351	HA	PRO A 541	-19.038	-0.548	-3.364	1.00	0.00
ATOM	352	IHB	PRO A 541	-16.851	-1.398	-3.438	1.00	0.00
ATOM	353	2HB	PRO A 541	-16.177	-0.009	-2.580	1.00	0.00
ATOM	354	IHG	PRO A 541	-15.486	0.569	-4.776	1.00	0.00
ATOM	355	2HG	PRO A 541	-16.837	-0.280	-5.532	1.00	0.00
ATOM	356	N	GLU A 542	-18.639	-0.749	-0.833	1.00	0.00
ATOM	357	CA	GLU A 542	-18.786	-0.718	0.588	1.00	0.00
ATOM	358	C	GLU A 542	-17.432	-0.466	1.160	1.00	0.00
ATOM	359	O	GLU A 542	-16.420	-0.621	0.479	1.00	0.00
ATOM	360	CB	GLU A 542	-19.285	-2.049	1.175	1.00	0.00
ATOM	361	CG	GLU A 542	-18.347	-3.227	0.897	1.00	0.00
ATOM	362	CD	GLU A 542	-18.417	-3.551	-0.591	1.00	0.00
ATOM	363	OE1	GLU A 542	-19.469	-3.240	-1.210	1.00	0.00
ATOM	364	OE2	GLU A 542	-17.422	-4.104	-1.128	1.00	0.00
ATOM	365	HN	GLU A 542	-18.654	-1.633	-1.300	1.00	0.00
ATOM	366	HA	GLU A 542	-19.496	0.078	0.809	1.00	0.00
ATOM	367	IHB	GLU A 542	-20.264	-2.273	0.751	1.00	0.00
ATOM	368	2HB	GLU A 542	-19.396	-1.937	2.253	1.00	0.00
ATOM	369	IHG	GLU A 542	-18.653	-4.102	1.470	1.00	0.00
ATOM	370	2HG	GLU A 542	-17.321	-2.969	1.160	1.00	0.00
ATOM	371	N	VAL A 543	-17.388	-0.040	2.437	1.00	0.00
ATOM	372	CA	VAL A 543	-16.125	0.195	3.068	1.00	0.00
ATOM	373	C	VAL A 543	-15.795	-1.069	3.786	1.00	0.00
ATOM	374	O	VAL A 543	-16.621	-1.625	4.509	1.00	0.00
ATOM	375	CB	VAL A 543	-16.144	1.314	4.072	1.00	0.00
ATOM	376	CG1	VAL A 543	-16.445	2.627	3.331	1.00	0.00
ATOM	377	CG2	VAL A 543	-17.163	0.980	5.175	1.00	0.00
ATOM	378	HN	VAL A 543	-18.237	0.111	2.944	1.00	0.00
ATOM	379	HA	VAL A 543	-15.421	0.427	2.269	1.00	0.00
ATOM	380	HB	VAL A 543	-15.179	1.381	4.574	1.00	0.00
ATOM	381	IHG1	VAL A 543	-17.412	2.575	2.831	1.00	0.00
ATOM	382	2HG1	VAL A 543	-15.684	2.816	2.575	1.00	0.00
ATOM	383	3HG1	VAL A 543	-16.475	3.458	4.036	1.00	0.00
ATOM	384	IHG2	VAL A 543	-16.736	0.284	5.896	1.00	0.00
ATOM	385	2HG2	VAL A 543	-18.048	0.516	4.741	1.00	0.00
ATOM	386	3HG2	VAL A 543	-17.449	1.886	5.709	1.00	0.00
ATOM	387	N	LEU A 544	-14.569	-1.575	3.578	1.00	0.00
ATOM	388	CA	LEU A 544	-14.209	-2.815	4.187	1.00	0.00
ATOM	389	C	LEU A 544	-13.656	-2.531	5.543	1.00	0.00
ATOM	390	O	LEU A 544	-13.348	-1.387	5.870	1.00	0.00
ATOM	391	CB	LEU A 544	-13.131	-3.564	3.395	1.00	0.00

24/208

ATOM	392	CG	LEU A 544	-13.493	-3.682	1.906	1.00	0.00
ATOM	393	CD1	LEU A 544	-13.254	-2.350	1.187	1.00	0.00
ATOM	394	CD2	LEU A 544	-12.800	-4.861	1.224	1.00	0.00
ATOM	395	HN	LEU A 544	-13.915	-1.086	3.001	1.00	0.00
ATOM	396	HA	LEU A 544	-15.118	-3.413	4.244	1.00	0.00
ATOM	397	1HB	LEU A 544	-13.010	-4.562	3.814	1.00	0.00
ATOM	398	2HB	LEU A 544	-12.184	-3.035	3.493	1.00	0.00
ATOM	399	HG	LEU A 544	-14.541	-3.965	1.807	1.00	0.00
ATOM	400	1HD1	LEU A 544	-12.442	-1.797	1.660	1.00	0.00
ATOM	401	2HD1	LEU A 544	-14.151	-1.732	1.230	1.00	0.00
ATOM	402	3HD1	LEU A 544	-12.980	-2.527	0.147	1.00	0.00
ATOM	403	1HD2	LEU A 544	-12.938	-5.775	1.802	1.00	0.00
ATOM	404	2HD2	LEU A 544	-11.729	-4.672	1.142	1.00	0.00
ATOM	405	3HD2	LEU A 544	-13.220	-5.022	0.232	1.00	0.00
ATOM	406	N	TYR A 545	-13.553	-3.581	6.380	1.00	0.00
ATOM	407	CA	TYR A 545	-12.972	-3.450	7.684	1.00	0.00
ATOM	408	C	TYR A 545	-11.713	-4.251	7.646	1.00	0.00
ATOM	409	O	TYR A 545	-11.640	-5.275	6.970	1.00	0.00
ATOM	410	CB	TYR A 545	-13.835	-4.014	8.827	1.00	0.00
ATOM	411	CG	TYR A 545	-14.981	-3.088	9.051	1.00	0.00
ATOM	412	CD1	TYR A 545	-14.854	-2.036	9.929	1.00	0.00
ATOM	413	CD2	TYR A 545	-16.172	-3.259	8.384	1.00	0.00
ATOM	414	CE1	TYR A 545	-15.902	-1.174	10.148	1.00	0.00
ATOM	415	CE2	TYR A 545	-17.220	-2.390	8.588	1.00	0.00
ATOM	416	CZ	TYR A 545	-17.085	-1.346	9.471	1.00	0.00
ATOM	417	OH	TYR A 545	-18.154	-0.448	9.677	1.00	0.00
ATOM	418	HN	TYR A 545	-13.890	-4.474	6.084	1.00	0.00
ATOM	419	HA	TYR A 545	-12.808	-2.384	7.838	1.00	0.00
ATOM	420	1HB	TYR A 545	-13.248	-4.092	9.742	1.00	0.00
ATOM	421	2HB	TYR A 545	-14.213	-5.002	8.566	1.00	0.00
ATOM	422	HD1	TYR A 545	-13.921	-1.887	10.453	1.00	0.00
ATOM	423	HE1	TYR A 545	-15.795	-0.361	10.851	1.00	0.00
ATOM	424	HD2	TYR A 545	-16.286	-4.081	7.693	1.00	0.00
ATOM	425	HE2	TYR A 545	-18.149	-2.530	8.055	1.00	0.00
ATOM	426	HH	TYR A 545	-17.937	0.394	9.299	1.00	0.00
ATOM	427	N	ALA A 546	-10.676	-3.791	8.370	1.00	0.00
ATOM	428	CA	ALA A 546	-9.426	-4.489	8.363	1.00	0.00
ATOM	429	C	ALA A 546	-9.603	-5.756	9.130	1.00	0.00
ATOM	430	O	ALA A 546	-10.566	-5.900	9.884	1.00	0.00
ATOM	431	CB	ALA A 546	-8.282	-3.699	9.022	1.00	0.00
ATOM	432	HN	ALA A 546	-10.780	-2.958	8.915	1.00	0.00
ATOM	433	HA	ALA A 546	-9.188	-4.688	7.318	1.00	0.00
ATOM	434	1HB	ALA A 546	-8.514	-3.481	10.064	1.00	0.00
ATOM	435	2HB	ALA A 546	-8.131	-2.752	8.505	1.00	0.00
ATOM	436	3HB	ALA A 546	-7.360	-4.281	8.998	1.00	0.00
ATOM	437	N	GLY A 547	-8.672	-6.714	8.923	1.00	0.00
ATOM	438	CA	GLY A 547	-8.686	-7.983	9.595	1.00	0.00
ATOM	439	C	GLY A 547	-8.822	-7.661	11.039	1.00	0.00
ATOM	440	O	GLY A 547	-8.298	-6.649	11.499	1.00	0.00

25/208

ATOM	441	HN	GLY A 547	-7.938	-6.529	8.269	1.00	0.00
ATOM	442	IHA	GLY A 547	-7.748	-8.499	9.398	1.00	0.00
ATOM	443	2HA	GLY A 547	-9.540	-8.560	9.243	1.00	0.00
ATOM	444	N	TYR A 548	-9.453	-8.584	11.790	1.00	0.00
ATOM	445	CA	TYR A 548	-9.937	-8.318	13.111	1.00	0.00
ATOM	446	C	TYR A 548	-8.940	-7.624	13.981	1.00	0.00
ATOM	447	O	TYR A 548	-9.107	-6.440	14.269	1.00	0.00
ATOM	448	CB	TYR A 548	-10.356	-9.629	13.804	1.00	0.00
ATOM	449	CG	TYR A 548	-11.182	-9.322	15.003	1.00	0.00
ATOM	450	CD1	TYR A 548	-12.506	-8.985	14.848	1.00	0.00
ATOM	451	CD2	TYR A 548	-10.694	-9.538	16.272	1.00	0.00
ATOM	452	CE1	TYR A 548	-13.324	-8.828	15.942	1.00	0.00
ATOM	453	CE2	TYR A 548	-11.507	-9.384	17.370	1.00	0.00
ATOM	454	CZ	TYR A 548	-12.825	-9.031	17.205	1.00	0.00
ATOM	455	OH	TYR A 548	-13.666	-8.889	18.330	1.00	0.00
ATOM	456	HN	TYR A 548	-9.589	-9.497	11.406	1.00	0.00
ATOM	457	HA	TYR A 548	-10.789	-7.645	13.015	1.00	0.00
ATOM	458	IHB	TYR A 548	-9.472	-10.187	14.114	1.00	0.00
ATOM	459	2HB	TYR A 548	-10.938	-10.245	13.118	1.00	0.00
ATOM	460	HD1	TYR A 548	-12.908	-8.841	13.856	1.00	0.00
ATOM	461	HE1	TYR A 548	-14.358	-8.545	15.808	1.00	0.00
ATOM	462	HD2	TYR A 548	-9.663	-9.831	16.406	1.00	0.00
ATOM	463	HE2	TYR A 548	-11.110	-9.540	18.362	1.00	0.00
ATOM	464	HH	TYR A 548	-13.522	-8.040	18.727	1.00	0.00
ATOM	465	N	ASP A 549	-7.850	-8.294	14.395	1.00	0.00
ATOM	466	CA	ASP A 549	-6.948	-7.558	15.232	1.00	0.00
ATOM	467	C	ASP A 549	-5.683	-8.324	15.365	1.00	0.00
ATOM	468	O	ASP A 549	-5.629	-9.359	16.027	1.00	0.00
ATOM	469	CB	ASP A 549	-7.494	-7.335	16.654	1.00	0.00
ATOM	470	CG	ASP A 549	-6.584	-6.355	17.379	1.00	0.00
ATOM	471	OD1	ASP A 549	-5.576	-5.914	16.766	1.00	0.00
ATOM	472	OD2	ASP A 549	-6.885	-6.035	18.561	1.00	0.00
ATOM	473	HN	ASP A 549	-7.680	-9.244	14.136	1.00	0.00
ATOM	474	HA	ASP A 549	-6.780	-6.599	14.742	1.00	0.00
ATOM	475	IHB	ASP A 549	-7.515	-8.276	17.204	1.00	0.00
ATOM	476	2HB	ASP A 549	-8.502	-6.924	16.613	1.00	0.00
ATOM	477	N	SER A 550	-4.609	-7.821	14.744	1.00	0.00
ATOM	478	CA	SER A 550	-3.373	-8.521	14.881	1.00	0.00
ATOM	479	C	SER A 550	-2.645	-7.794	15.955	1.00	0.00
ATOM	480	O	SER A 550	-3.151	-6.823	16.517	1.00	0.00
ATOM	481	CB	SER A 550	-2.526	-8.504	13.598	1.00	0.00
ATOM	482	OG	SER A 550	-1.473	-9.449	13.698	1.00	0.00
ATOM	483	HN	SER A 550	-4.671	-6.983	14.202	1.00	0.00
ATOM	484	HA	SER A 550	-3.625	-9.547	15.149	1.00	0.00
ATOM	485	IHB	SER A 550	-2.088	-7.518	13.447	1.00	0.00
ATOM	486	2HB	SER A 550	-3.140	-8.766	12.736	1.00	0.00
ATOM	487	HG	SER A 550	-0.895	-9.291	12.962	1.00	0.00
ATOM	488	N	SER A 551	-1.439	-8.267	16.297	1.00	0.00
ATOM	489	CA	SER A 551	-0.702	-7.585	17.309	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

26/208

ATOM	490	C	SER A 551	-0.469	-6.217	16.768	1.00	0.00
ATOM	491	O	SER A 551	0.342	-6.026	15.864	1.00	0.00
ATOM	492	CB	SER A 551	0.641	-8.274	17.608	1.00	0.00
ATOM	493	OG	SER A 551	1.360	-7.589	18.614	1.00	0.00
ATOM	494	HN	SER A 551	-1.064	-9.080	15.851	1.00	0.00
ATOM	495	HA	SER A 551	-1.328	-7.572	18.202	1.00	0.00
ATOM	496	IHB	SER A 551	1.258	-8.293	16.710	1.00	0.00
ATOM	497	2HB	SER A 551	0.469	-9.293	17.954	1.00	0.00
ATOM	498	HG	SER A 551	2.271	-7.596	18.352	1.00	0.00
ATOM	499	N	VAL A 552	-1.170	-5.219	17.339	1.00	0.00
ATOM	500	CA	VAL A 552	-1.031	-3.881	16.855	1.00	0.00
ATOM	501	C	VAL A 552	0.410	-3.529	16.975	1.00	0.00
ATOM	502	O	VAL A 552	0.852	-2.649	16.236	1.00	0.00
ATOM	503	CB	VAL A 552	-1.932	-2.839	17.492	1.00	0.00
ATOM	504	CG1	VAL A 552	-1.754	-2.760	19.016	1.00	0.00
ATOM	505	CG2	VAL A 552	-1.651	-1.508	16.776	1.00	0.00
ATOM	506	HN	VAL A 552	-1.786	-5.414	18.102	1.00	0.00
ATOM	507	HA	VAL A 552	-1.238	-3.931	15.787	1.00	0.00
ATOM	508	HB	VAL A 552	-2.970	-3.084	17.269	1.00	0.00
ATOM	509	IHG1	VAL A 552	-0.784	-2.330	19.269	1.00	0.00
ATOM	510	2HG1	VAL A 552	-1.805	-3.757	19.454	1.00	0.00
ATOM	511	3HG1	VAL A 552	-2.526	-2.127	19.453	1.00	0.00
ATOM	512	IHG2	VAL A 552	-1.522	-1.666	15.705	1.00	0.00
ATOM	513	2HG2	VAL A 552	-0.738	-1.057	17.163	1.00	0.00
ATOM	514	3HG2	VAL A 552	-2.487	-0.821	16.916	1.00	0.00
ATOM	515	N	PRO A 553	1.160	-4.153	17.874	1.00	0.00
ATOM	516	CA	PRO A 553	2.572	-3.997	17.780	1.00	0.00
ATOM	517	C	PRO A 553	2.839	-4.634	16.475	1.00	0.00
ATOM	518	O	PRO A 553	2.831	-5.855	16.329	1.00	0.00
ATOM	519	CB	PRO A 553	3.197	-4.627	19.024	1.00	0.00
ATOM	520	CG	PRO A 553	1.990	-5.107	19.854	1.00	0.00
ATOM	521	CD	PRO A 553	0.789	-4.348	19.267	1.00	0.00
ATOM	522	IHD	PRO A 553	-0.128	-4.931	19.343	1.00	0.00
ATOM	523	2HD	PRO A 553	0.641	-3.389	19.764	1.00	0.00
ATOM	524	HA	PRO A 553	2.820	-2.936	17.724	1.00	0.00
ATOM	525	IHB	PRO A 553	3.789	-3.899	19.578	1.00	0.00
ATOM	526	2HB	PRO A 553	3.846	-5.461	18.758	1.00	0.00
ATOM	527	IHG	PRO A 553	1.855	-6.185	19.760	1.00	0.00
ATOM	528	2HG	PRO A 553	2.123	-4.872	20.910	1.00	0.00
ATOM	529	N	ASP A 554	3.070	-3.759	15.508	1.00	0.00
ATOM	530	CA	ASP A 554	3.109	-4.093	14.145	1.00	0.00
ATOM	531	C	ASP A 554	4.536	-4.346	13.841	1.00	0.00
ATOM	532	O	ASP A 554	5.427	-3.941	14.583	1.00	0.00
ATOM	533	CB	ASP A 554	2.635	-2.882	13.334	1.00	0.00
ATOM	534	CG	ASP A 554	1.951	-3.364	12.080	1.00	0.00
ATOM	535	OD1	ASP A 554	1.372	-2.506	11.363	1.00	0.00
ATOM	536	OD2	ASP A 554	1.967	-4.600	11.845	1.00	0.00
ATOM	537	HN	ASP A 554	3.225	-2.805	15.764	1.00	0.00
ATOM	538	HA	ASP A 554	2.451	-4.948	13.993	1.00	0.00

27/208

ATOM	539	IHB	ASP A 554	3.485	-2.257	13.058	1.00	0.00
ATOM	540	2HB	ASP A 554	1.931	-2.288	13.917	1.00	0.00
ATOM	541	N	SER A 555	4.776	-5.073	12.743	1.00	0.00
ATOM	542	CA	SER A 555	6.104	-5.349	12.312	1.00	0.00
ATOM	543	C	SER A 555	6.030	-5.073	10.856	1.00	0.00
ATOM	544	O	SER A 555	4.938	-4.848	10.338	1.00	0.00
ATOM	545	CB	SER A 555	6.514	-6.816	12.521	1.00	0.00
ATOM	546	OG	SER A 555	5.603	-7.675	11.852	1.00	0.00
ATOM	547	HN	SER A 555	4.005	-5.430	12.216	1.00	0.00
ATOM	548	HA	SER A 555	6.759	-4.692	12.884	1.00	0.00
ATOM	549	IHB	SER A 555	6.503	-7.065	13.582	1.00	0.00
ATOM	550	2HB	SER A 555	7.511	-6.991	12.116	1.00	0.00
ATOM	551	HG	SER A 555	5.751	-7.557	10.923	1.00	0.00
ATOM	552	N	THR A 556	7.183	-5.076	10.161	1.00	0.00
ATOM	553	CA	THR A 556	7.172	-4.781	8.758	1.00	0.00
ATOM	554	C	THR A 556	6.244	-5.759	8.124	1.00	0.00
ATOM	555	O	THR A 556	5.354	-5.390	7.362	1.00	0.00
ATOM	556	CB	THR A 556	8.511	-4.981	8.118	1.00	0.00
ATOM	557	OG1	THR A 556	9.474	-4.118	8.704	1.00	0.00
ATOM	558	CG2	THR A 556	8.382	-4.706	6.612	1.00	0.00
ATOM	559	HN	THR A 556	8.045	-5.284	10.623	1.00	0.00
ATOM	560	HA	THR A 556	6.860	-3.741	8.659	1.00	0.00
ATOM	561	HB	THR A 556	8.845	-6.009	8.258	1.00	0.00
ATOM	562	HG1	THR A 556	9.460	-3.314	8.202	1.00	0.00
ATOM	563	IHG2	THR A 556	7.884	-3.753	6.435	1.00	0.00
ATOM	564	2HG2	THR A 556	7.791	-5.488	6.135	1.00	0.00
ATOM	565	3HG2	THR A 556	9.369	-4.661	6.152	1.00	0.00
ATOM	566	N	TRP A 557	6.412	-7.044	8.467	1.00	0.00
ATOM	567	CA	TRP A 557	5.573	-8.072	7.932	1.00	0.00
ATOM	568	C	TRP A 557	4.169	-7.891	8.395	1.00	0.00
ATOM	569	O	TRP A 557	3.224	-7.991	7.617	1.00	0.00
ATOM	570	CB	TRP A 557	5.970	-9.465	8.426	1.00	0.00
ATOM	571	CG	TRP A 557	7.251	-9.979	7.837	1.00	0.00
ATOM	572	CD1	TRP A 557	7.419	-10.886	6.838	1.00	0.00
ATOM	573	CD2	TRP A 557	8.561	-9.507	8.186	1.00	0.00
ATOM	574	NE1	TRP A 557	8.755	-11.037	6.572	1.00	0.00
ATOM	575	CE2	TRP A 557	9.468	-10.184	7.380	1.00	0.00
ATOM	576	CE3	TRP A 557	8.975	-8.580	9.100	1.00	0.00
ATOM	577	CZ2	TRP A 557	10.812	-9.953	7.466	1.00	0.00
ATOM	578	CZ3	TRP A 557	10.331	-8.349	9.190	1.00	0.00
ATOM	579	CH2	TRP A 557	11.232	-9.022	8.391	1.00	0.00
ATOM	580	HN	TRP A 557	7.138	-7.288	9.111	1.00	0.00
ATOM	581	HA	TRP A 557	5.663	-8.018	6.847	1.00	0.00
ATOM	582	IHB	TRP A 557	5.178	-10.169	8.173	1.00	0.00
ATOM	583	2HB	TRP A 557	6.086	-9.437	9.509	1.00	0.00
ATOM	584	HE3	TRP A 557	8.270	-8.051	9.724	1.00	0.00
ATOM	585	HD1	TRP A 557	6.621	-11.408	6.331	1.00	0.00
ATOM	586	HE1	TRP A 557	9.139	-11.653	5.914	1.00	0.00
ATOM	587	HZ2	TRP A 557	11.514	-10.477	6.836	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

28/208

ATOM	588	HZ3 TRP A 557	10.696	-7.625	9.903	1.00	0.00
ATOM	589	HH2 TRP A 557	12.287	-8.814	8.492	1.00	0.00
ATOM	590	N ARG A 558	4.005	-7.601	9.693	1.00	0.00
ATOM	591	CA ARG A 558	2.695	-7.561	10.258	1.00	0.00
ATOM	592	C ARG A 558	1.909	-6.485	9.583	1.00	0.00
ATOM	593	O ARG A 558	0.749	-6.681	9.224	1.00	0.00
ATOM	594	CB ARG A 558	2.762	-7.263	11.763	1.00	0.00
ATOM	595	CG ARG A 558	1.578	-7.783	12.573	1.00	0.00
ATOM	596	CD ARG A 558	1.839	-7.698	14.077	1.00	0.00
ATOM	597	NE ARG A 558	0.831	-8.545	14.771	1.00	0.00
ATOM	598	CZ ARG A 558	1.075	-9.869	14.997	1.00	0.00
ATOM	599	NH1 ARG A 558	2.205	-10.454	14.502	1.00	0.00
ATOM	600	NH2 ARG A 558	0.195	-10.607	15.736	1.00	0.00
ATOM	601	HN ARG A 558	4.803	-7.413	10.266	1.00	0.00
ATOM	602	HA ARG A 558	2.236	-8.533	10.079	1.00	0.00
ATOM	603	IHB ARG A 558	2.822	-6.184	11.897	1.00	0.00
ATOM	604	2HB ARG A 558	3.672	-7.710	12.161	1.00	0.00
ATOM	605	IHG ARG A 558	1.386	-8.820	12.301	1.00	0.00
ATOM	606	2HG ARG A 558	0.693	-7.196	12.330	1.00	0.00
ATOM	607	IHD ARG A 558	1.725	-6.677	14.440	1.00	0.00
ATOM	608	2HD ARG A 558	2.827	-8.082	14.328	1.00	0.00
ATOM	609	HE ARG A 558	-0.032	-8.142	15.074	1.00	0.00
ATOM	610	1HH1 ARG A 558	2.857	-9.913	13.970	1.00	0.00
ATOM	611	2HH1 ARG A 558	2.379	-11.425	14.670	1.00	0.00
ATOM	612	1HH2 ARG A 558	-0.745	-10.289	15.857	1.00	0.00
ATOM	613	2HH2 ARG A 558	0.491	-11.465	16.155	1.00	0.00
ATOM	614	N ILE A 559	2.516	-5.305	9.292	1.00	0.00
ATOM	615	CA ILE A 559	1.827	-4.119	8.731	1.00	0.00
ATOM	616	C ILE A 559	1.497	-4.396	7.283	1.00	0.00
ATOM	617	O ILE A 559	0.366	-4.265	6.822	1.00	0.00
ATOM	618	CB ILE A 559	2.656	-2.787	8.783	1.00	0.00
ATOM	619	CG1 ILE A 559	1.967	-1.560	8.132	1.00	0.00
ATOM	620	CG2 ILE A 559	4.060	-2.914	8.240	1.00	0.00
ATOM	621	CD1 ILE A 559	0.721	-1.051	8.861	1.00	0.00
ATOM	622	HN ILE A 559	3.453	-5.200	9.578	1.00	0.00
ATOM	623	HA ILE A 559	0.895	-4.007	9.286	1.00	0.00
ATOM	624	HB ILE A 559	2.893	-2.543	9.804	1.00	0.00
ATOM	625	IHG2 ILE A 559	4.120	-2.765	7.164	1.00	0.00
ATOM	626	2HG2 ILE A 559	4.412	-3.883	8.472	1.00	0.00
ATOM	627	3HG2 ILE A 559	4.748	-2.270	8.777	1.00	0.00
ATOM	628	IHG1 ILE A 559	1.714	-1.773	7.093	1.00	0.00
ATOM	629	2HG1 ILE A 559	2.672	-0.731	8.090	1.00	0.00
ATOM	630	IHD1 ILE A 559	-0.007	-1.846	9.020	1.00	0.00
ATOM	631	2HD1 ILE A 559	0.242	-0.254	8.293	1.00	0.00
ATOM	632	3HD1 ILE A 559	0.983	-0.634	9.833	1.00	0.00
ATOM	633	N MET A 560	2.586	-4.806	6.598	1.00	0.00
ATOM	634	CA MET A 560	2.513	-5.064	5.177	1.00	0.00
ATOM	635	C MET A 560	1.384	-6.043	4.913	1.00	0.00
ATOM	636	O MET A 560	0.660	-5.940	3.937	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

29/208

ATOM	637	CB	MET A 560	3.840	-5.628	4.656	1.00	0.00
ATOM	638	CG	MET A 560	3.772	-5.929	3.156	1.00	0.00
ATOM	639	SD	MET A 560	3.305	-4.449	2.226	1.00	0.00
ATOM	640	CE	MET A 560	2.780	-5.201	0.678	1.00	0.00
ATOM	641	HN	MET A 560	3.463	-4.907	7.078	1.00	0.00
ATOM	642	HA	MET A 560	2.274	-4.111	4.702	1.00	0.00
ATOM	643	IHB	MET A 560	4.106	-6.536	5.201	1.00	0.00
ATOM	644	2HB	MET A 560	4.639	-4.912	4.848	1.00	0.00
ATOM	645	IHG	MET A 560	3.035	-6.709	2.967	1.00	0.00
ATOM	646	2HG	MET A 560	4.718	-6.332	2.808	1.00	0.00
ATOM	647	IHE	MET A 560	3.583	-5.175	-0.059	1.00	0.00
ATOM	648	2HE	MET A 560	1.926	-4.659	0.276	1.00	0.00
ATOM	649	3HE	MET A 560	2.462	-6.227	0.842	1.00	0.00
ATOM	650	N	THR A 561	1.254	-6.972	5.877	1.00	0.00
ATOM	651	CA	THR A 561	0.230	-7.957	5.717	1.00	0.00
ATOM	652	C	THR A 561	-1.132	-7.338	5.753	1.00	0.00
ATOM	653	O	THR A 561	-1.942	-7.591	4.863	1.00	0.00
ATOM	654	CB	THR A 561	0.253	-9.015	6.778	1.00	0.00
ATOM	655	OG1	THR A 561	-1.491	-9.710	6.754	1.00	0.00
ATOM	656	CG2	THR A 561	-0.907	-9.991	6.513	1.00	0.00
ATOM	657	HN	THR A 561	1.885	-7.023	6.651	1.00	0.00
ATOM	658	HA	THR A 561	0.384	-8.408	4.737	1.00	0.00
ATOM	659	HB	THR A 561	0.134	-8.564	7.763	1.00	0.00
ATOM	660	HG1	THR A 561	2.165	-9.061	6.598	1.00	0.00
ATOM	661	IHG2	THR A 561	-1.011	-10.185	5.445	1.00	0.00
ATOM	662	2HG2	THR A 561	-1.845	-9.567	6.872	1.00	0.00
ATOM	663	3HG2	THR A 561	-0.720	-10.942	7.012	1.00	0.00
ATOM	664	N	THR A 562	-1.371	-6.504	6.773	1.00	0.00
ATOM	665	CA	THR A 562	-2.671	-5.876	6.947	1.00	0.00
ATOM	666	C	THR A 562	-3.073	-5.043	5.712	1.00	0.00
ATOM	667	O	THR A 562	-4.151	-5.207	5.157	1.00	0.00
ATOM	668	CB	THR A 562	-2.575	-5.035	8.237	1.00	0.00
ATOM	669	OG1	THR A 562	-2.067	-5.838	9.297	1.00	0.00
ATOM	670	CG2	THR A 562	-3.945	-4.514	8.686	1.00	0.00
ATOM	671	HN	THR A 562	-0.606	-6.273	7.377	1.00	0.00
ATOM	672	HA	THR A 562	-3.391	-6.686	7.073	1.00	0.00
ATOM	673	HB	THR A 562	-1.920	-4.166	8.084	1.00	0.00
ATOM	674	HG1	THR A 562	-1.128	-6.023	9.203	1.00	0.00
ATOM	675	IHG2	THR A 562	-4.389	-3.856	7.939	1.00	0.00
ATOM	676	2HG2	THR A 562	-3.856	-3.947	9.613	1.00	0.00
ATOM	677	3HG2	THR A 562	-4.638	-5.336	8.866	1.00	0.00
ATOM	678	N	LEU A 563	-2.142	-4.157	5.310	1.00	0.00
ATOM	679	CA	LEU A 563	-2.440	-3.258	4.196	1.00	0.00
ATOM	680	C	LEU A 563	-2.561	-4.047	2.878	1.00	0.00
ATOM	681	O	LEU A 563	-3.452	-3.801	2.073	1.00	0.00
ATOM	682	CB	LEU A 563	-1.381	-2.149	4.098	1.00	0.00
ATOM	683	CG	LEU A 563	-1.569	-0.984	5.091	1.00	0.00
ATOM	684	CD1	LEU A 563	-1.720	-1.439	6.549	1.00	0.00
ATOM	685	CD2	LEU A 563	-0.413	0.017	4.954	1.00	0.00

30/208

ATOM	686	HN	LEU A 563	-1.264	-4.106	5.796	1.00	0.00
ATOM	687	HA	LEU A 563	-3.410	-2.801	4.390	1.00	0.00
ATOM	688	1HB	LEU A 563	-1.439	-1.707	3.105	1.00	0.00
ATOM	689	2HB	LEU A 563	-0.382	-2.579	4.191	1.00	0.00
ATOM	690	HG	LEU A 563	-2.487	-0.461	4.821	1.00	0.00
ATOM	691	1HD1	LEU A 563	-0.876	-2.055	6.857	1.00	0.00
ATOM	692	2HD1	LEU A 563	-2.635	-2.010	6.700	1.00	0.00
ATOM	693	3HD1	LEU A 563	-1.775	-0.581	7.219	1.00	0.00
ATOM	694	1HD2	LEU A 563	-0.560	0.881	5.602	1.00	0.00
ATOM	695	2HD2	LEU A 563	-0.326	0.384	3.930	1.00	0.00
ATOM	696	3HD2	LEU A 563	0.540	-0.440	5.222	1.00	0.00
ATOM	697	N	ASN A 564	-1.646	-5.027	2.717	1.00	0.00
ATOM	698	CA	ASN A 564	-1.710	-5.941	1.569	1.00	0.00
ATOM	699	C	ASN A 564	-3.102	-6.582	1.520	1.00	0.00
ATOM	700	O	ASN A 564	-3.801	-6.536	0.512	1.00	0.00
ATOM	701	CB	ASN A 564	-0.592	-7.011	1.653	1.00	0.00
ATOM	702	CG	ASN A 564	-0.641	-8.077	0.538	1.00	0.00
ATOM	703	OD1	ASN A 564	-1.700	-8.457	0.065	1.00	0.00
ATOM	704	ND2	ASN A 564	0.545	-8.582	0.169	1.00	0.00
ATOM	705	HN	ASN A 564	-0.928	-5.159	3.402	1.00	0.00
ATOM	706	HA	ASN A 564	-1.582	-5.330	0.675	1.00	0.00
ATOM	707	1HB	ASN A 564	-0.651	-7.542	2.602	1.00	0.00
ATOM	708	2HB	ASN A 564	0.379	-6.522	1.619	1.00	0.00
ATOM	709	1HD2	ASN A 564	0.559	-9.377	-0.441	1.00	0.00
ATOM	710	2HD2	ASN A 564	1.444	-8.223	0.435	1.00	0.00
ATOM	711	N	MET A 565	-3.472	-7.139	2.692	1.00	0.00
ATOM	712	CA	MET A 565	-4.686	-7.899	2.761	1.00	0.00
ATOM	713	C	MET A 565	-5.855	-7.025	2.425	1.00	0.00
ATOM	714	O	MET A 565	-6.733	-7.428	1.664	1.00	0.00
ATOM	715	CB	MET A 565	-4.937	-8.481	4.163	1.00	0.00
ATOM	716	CG	MET A 565	-3.928	-9.557	4.569	1.00	0.00
ATOM	717	SD	MET A 565	-4.074	-11.110	3.635	1.00	0.00
ATOM	718	CE	MET A 565	-5.609	-11.633	4.455	1.00	0.00
ATOM	719	HN	MET A 565	-2.938	-6.992	3.525	1.00	0.00
ATOM	720	HA	MET A 565	-4.595	-8.703	2.030	1.00	0.00
ATOM	721	1HB	MET A 565	-5.937	-8.912	4.188	1.00	0.00
ATOM	722	2HB	MET A 565	-4.895	-7.671	4.890	1.00	0.00
ATOM	723	1HG	MET A 565	-4.066	-9.787	5.625	1.00	0.00
ATOM	724	2HG	MET A 565	-2.921	-9.170	4.419	1.00	0.00
ATOM	725	1HE	MET A 565	-6.429	-10.989	4.136	1.00	0.00
ATOM	726	2HE	MET A 565	-5.500	-11.548	5.536	1.00	0.00
ATOM	727	3HE	MET A 565	-5.845	-12.660	4.178	1.00	0.00
ATOM	728	N	LEU A 566	-5.845	-5.812	3.021	1.00	0.00
ATOM	729	CA	LEU A 566	-6.856	-4.788	2.773	1.00	0.00
ATOM	730	C	LEU A 566	-7.043	-4.576	1.264	1.00	0.00
ATOM	731	O	LEU A 566	-8.154	-4.613	0.750	1.00	0.00
ATOM	732	CB	LEU A 566	-6.464	-3.475	3.487	1.00	0.00
ATOM	733	CG	LEU A 566	-6.893	-3.414	4.968	1.00	0.00
ATOM	734	CD1	LEU A 566	-5.988	-2.478	5.781	1.00	0.00



31/208

ATOM	735	CD2 LEU A 566	-8.353	-2.956	5.095	1.00	0.00
ATOM	736	HN LEU A 566	-5.087	-5.613	3.643	1.00	0.00
ATOM	737	HA LEU A 566	-7.791	-5.160	3.176	1.00	0.00
ATOM	738	1HB LEU A 566	-6.893	-2.613	2.973	1.00	0.00
ATOM	739	2HB LEU A 566	-5.388	-3.342	3.410	1.00	0.00
ATOM	740	HG LEU A 566	-6.798	-4.408	5.407	1.00	0.00
ATOM	741	1HD1 LEU A 566	-4.981	-2.879	5.866	1.00	0.00
ATOM	742	2HD1 LEU A 566	-6.363	-2.343	6.796	1.00	0.00
ATOM	743	3HD1 LEU A 566	-5.914	-1.497	5.316	1.00	0.00
ATOM	744	1HD2 LEU A 566	-8.650	-2.858	6.138	1.00	0.00
ATOM	745	2HD2 LEU A 566	-9.029	-3.662	4.622	1.00	0.00
ATOM	746	3HD2 LEU A 566	-8.503	-1.982	4.627	1.00	0.00
ATOM	747	N GLY A 567	-5.891	-4.374	0.598	1.00	0.00
ATOM	748	CA GLY A 567	-5.899	-4.129	-0.841	1.00	0.00
ATOM	749	C GLY A 567	-6.516	-5.286	-1.627	1.00	0.00
ATOM	750	O GLY A 567	-7.377	-5.103	-2.480	1.00	0.00
ATOM	751	HN GLY A 567	-5.023	-4.395	1.103	1.00	0.00
ATOM	752	1HA GLY A 567	-4.867	-3.974	-1.156	1.00	0.00
ATOM	753	2HA GLY A 567	-6.481	-3.231	-1.031	1.00	0.00
ATOM	754	N GLY A 568	-6.043	-6.488	-1.267	1.00	0.00
ATOM	755	CA GLY A 568	-6.495	-7.693	-1.948	1.00	0.00
ATOM	756	C GLY A 568	-8.001	-7.959	-1.776	1.00	0.00
ATOM	757	O GLY A 568	-8.615	-8.640	-2.582	1.00	0.00
ATOM	758	HN GLY A 568	-5.345	-6.546	-0.547	1.00	0.00
ATOM	759	1HA GLY A 568	-5.925	-8.524	-1.533	1.00	0.00
ATOM	760	2HA GLY A 568	-6.253	-7.593	-3.007	1.00	0.00
ATOM	761	N ARG A 569	-8.568	-7.380	-0.701	1.00	0.00
ATOM	762	CA ARG A 569	-9.988	-7.439	-0.493	1.00	0.00
ATOM	763	C ARG A 569	-10.710	-6.424	-1.328	1.00	0.00
ATOM	764	O ARG A 569	-11.707	-6.727	-1.980	1.00	0.00
ATOM	765	CB ARG A 569	-10.338	-7.144	0.977	1.00	0.00
ATOM	766	CG ARG A 569	-9.768	-8.193	1.934	1.00	0.00
ATOM	767	CD ARG A 569	-9.594	-7.720	3.379	1.00	0.00
ATOM	768	NE ARG A 569	-10.941	-7.532	3.984	1.00	0.00
ATOM	769	CZ ARG A 569	-11.478	-6.280	4.060	1.00	0.00
ATOM	770	NH1 ARG A 569	-10.793	-5.217	3.548	1.00	0.00
ATOM	771	NH2 ARG A 569	-12.689	-6.097	4.662	1.00	0.00
ATOM	772	HN ARG A 569	-7.980	-7.066	0.045	1.00	0.00
ATOM	773	HA ARG A 569	-10.314	-8.441	-0.770	1.00	0.00
ATOM	774	1HB ARG A 569	-11.422	-7.116	1.085	1.00	0.00
ATOM	775	2HB ARG A 569	-9.943	-6.165	1.246	1.00	0.00
ATOM	776	1HG ARG A 569	-8.796	-8.508	1.557	1.00	0.00
ATOM	777	2HG ARG A 569	-10.432	-9.055	1.932	1.00	0.00
ATOM	778	1HD ARG A 569	-9.077	-6.762	3.419	1.00	0.00
ATOM	779	2HD ARG A 569	-9.064	-8.463	3.974	1.00	0.00
ATOM	780	HE ARG A 569	-11.450	-8.319	4.333	1.00	0.00
ATOM	781	1HH1 ARG A 569	-9.901	-5.357	3.119	1.00	0.00
ATOM	782	2HH1 ARG A 569	-11.184	-4.298	3.602	1.00	0.00
ATOM	783	1HH2 ARG A 569	-12.893	-5.232	5.122	1.00	0.00

32/208

ATOM	784	2HH2 ARG A 569	-13.372	-6.827	4.644	1.00	0.00
ATOM	785	N GLN A 570	-10.148	-5.202	-1.264	1.00	0.00
ATOM	786	CA GLN A 570	-10.705	-4.047	-1.949	1.00	0.00
ATOM	787	C GLN A 570	-10.795	-4.290	-3.471	1.00	0.00
ATOM	788	O GLN A 570	-11.690	-3.789	-4.138	1.00	0.00
ATOM	789	CB GLN A 570	-9.800	-2.832	-1.665	1.00	0.00
ATOM	790	CG GLN A 570	-9.791	-2.333	-0.204	1.00	0.00
ATOM	791	CD GLN A 570	-10.411	-0.934	-0.079	1.00	0.00
ATOM	792	OE1 GLN A 570	-11.507	-0.680	-0.549	1.00	0.00
ATOM	793	NE2 GLN A 570	-9.663	-0.034	0.566	1.00	0.00
ATOM	794	HN GLN A 570	-9.315	-5.093	-0.714	1.00	0.00
ATOM	795	HA GLN A 570	-11.711	-3.886	-1.560	1.00	0.00
ATOM	796	IHB GLN A 570	-10.072	-2.022	-2.342	1.00	0.00
ATOM	797	2HB GLN A 570	-8.776	-3.100	-1.915	1.00	0.00
ATOM	798	IHG GLN A 570	-8.767	-2.289	0.165	1.00	0.00
ATOM	799	2HG GLN A 570	-10.334	-3.011	0.452	1.00	0.00
ATOM	800	IHE2 GLN A 570	-8.752	-0.195	0.949	1.00	0.00
ATOM	801	2HE2 GLN A 570	-10.037	0.888	0.666	1.00	0.00
ATOM	802	N VAL A 571	-9.829	-5.086	-3.988	1.00	0.00
ATOM	803	CA VAL A 571	-9.746	-5.296	-5.400	1.00	0.00
ATOM	804	C VAL A 571	-10.979	-5.988	-5.885	1.00	0.00
ATOM	805	O VAL A 571	-11.453	-5.695	-6.980	1.00	0.00
ATOM	806	CB VAL A 571	-8.564	-6.113	-5.838	1.00	0.00
ATOM	807	CG1 VAL A 571	-8.809	-7.579	-5.465	1.00	0.00
ATOM	808	CG2 VAL A 571	-8.355	-5.896	-7.346	1.00	0.00
ATOM	809	HN VAL A 571	-9.145	-5.485	-3.377	1.00	0.00
ATOM	810	HA VAL A 571	-9.697	-4.306	-5.853	1.00	0.00
ATOM	811	HB VAL A 571	-7.661	-5.751	-5.347	1.00	0.00
ATOM	812	IHG1 VAL A 571	-9.464	-8.058	-6.194	1.00	0.00
ATOM	813	2HG1 VAL A 571	-9.288	-7.645	-4.488	1.00	0.00
ATOM	814	3HG1 VAL A 571	-7.866	-8.126	-5.449	1.00	0.00
ATOM	815	IHG2 VAL A 571	-8.168	-4.845	-7.562	1.00	0.00
ATOM	816	2HG2 VAL A 571	-9.245	-6.200	-7.897	1.00	0.00
ATOM	817	3HG2 VAL A 571	-7.496	-6.470	-7.693	1.00	0.00
ATOM	818	N ILE A 572	-11.533	-6.934	-5.099	1.00	0.00
ATOM	819	CA ILE A 572	-12.701	-7.619	-5.569	1.00	0.00
ATOM	820	C ILE A 572	-13.819	-6.633	-5.718	1.00	0.00
ATOM	821	O ILE A 572	-14.523	-6.622	-6.725	1.00	0.00
ATOM	822	CB ILE A 572	-13.177	-8.716	-4.653	1.00	0.00
ATOM	823	CG1 ILE A 572	-13.637	-8.160	-3.296	1.00	0.00
ATOM	824	CG2 ILE A 572	-12.047	-9.754	-4.539	1.00	0.00
ATOM	825	CD1 ILE A 572	-14.406	-9.173	-2.447	1.00	0.00
ATOM	826	HN ILE A 572	-11.136	-7.152	-4.207	1.00	0.00
ATOM	827	HA ILE A 572	-12.442	-8.035	-6.542	1.00	0.00
ATOM	828	HB ILE A 572	-14.076	-9.181	-5.057	1.00	0.00
ATOM	829	IHG2 ILE A 572	-11.145	-9.299	-4.131	1.00	0.00
ATOM	830	2HG2 ILE A 572	-11.806	-10.157	-5.523	1.00	0.00
ATOM	831	3HG2 ILE A 572	-12.346	-10.564	-3.874	1.00	0.00
ATOM	832	IHG1 ILE A 572	-14.276	-7.296	-3.471	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

33/208

ATOM	833	2HG1 ILE A 572	-12.761	-7.831	-2.738	1.00	0.00
ATOM	834	1HD1 ILE A 572	-13.787	-10.046	-2.234	1.00	0.00
ATOM	835	2HD1 ILE A 572	-15.295	-9.512	-2.978	1.00	0.00
ATOM	836	3HD1 ILE A 572	-14.695	-8.726	-1.496	1.00	0.00
ATOM	837	N ALA A 573	-13.995	-5.749	-4.721	1.00	0.00
ATOM	838	CA ALA A 573	-15.062	-4.793	-4.764	1.00	0.00
ATOM	839	C ALA A 573	-14.833	-3.877	-5.920	1.00	0.00
ATOM	840	O ALA A 573	-15.775	-3.457	-6.590	1.00	0.00
ATOM	841	CB ALA A 573	-15.137	-3.928	-3.494	1.00	0.00
ATOM	842	HN ALA A 573	-13.372	-5.759	-3.939	1.00	0.00
ATOM	843	HA ALA A 573	-15.985	-5.359	-4.888	1.00	0.00
ATOM	844	1HB ALA A 573	-14.292	-3.242	-3.444	1.00	0.00
ATOM	845	2HB ALA A 573	-15.110	-4.560	-2.606	1.00	0.00
ATOM	846	3HB ALA A 573	-16.052	-3.336	-3.495	1.00	0.00
ATOM	847	N ALA A 574	-13.554	-3.564	-6.190	1.00	0.00
ATOM	848	CA ALA A 574	-13.203	-2.632	-7.220	1.00	0.00
ATOM	849	C ALA A 574	-13.693	-3.097	-8.553	1.00	0.00
ATOM	850	O ALA A 574	-14.242	-2.312	-9.323	1.00	0.00
ATOM	851	CB ALA A 574	-11.683	-2.427	-7.337	1.00	0.00
ATOM	852	HN ALA A 574	-12.827	-3.994	-5.655	1.00	0.00
ATOM	853	HA ALA A 574	-13.691	-1.690	-6.971	1.00	0.00
ATOM	854	1HB ALA A 574	-11.184	-3.368	-7.569	1.00	0.00
ATOM	855	2HB ALA A 574	-11.280	-2.055	-6.395	1.00	0.00
ATOM	856	3HB ALA A 574	-11.459	-1.721	-8.137	1.00	0.00
ATOM	857	N VAL A 575	-13.530	-4.399	-8.853	1.00	0.00
ATOM	858	CA VAL A 575	-13.925	-4.888	-10.141	1.00	0.00
ATOM	859	C VAL A 575	-15.398	-4.687	-10.298	1.00	0.00
ATOM	860	O VAL A 575	-15.870	-4.340	-11.381	1.00	0.00
ATOM	861	CB VAL A 575	-13.632	-6.348	-10.347	1.00	0.00
ATOM	862	CG1 VAL A 575	-14.518	-7.183	-9.409	1.00	0.00
ATOM	863	CG2 VAL A 575	-13.839	-6.673	-11.835	1.00	0.00
ATOM	864	HN VAL A 575	-13.134	-5.023	-8.179	1.00	0.00
ATOM	865	HA VAL A 575	-13.384	-4.293	-10.877	1.00	0.00
ATOM	866	HB VAL A 575	-12.581	-6.547	-10.136	1.00	0.00
ATOM	867	1HG1 VAL A 575	-15.377	-7.584	-9.947	1.00	0.00
ATOM	868	2HG1 VAL A 575	-14.890	-6.565	-8.592	1.00	0.00
ATOM	869	3HG1 VAL A 575	-13.952	-8.023	-9.005	1.00	0.00
ATOM	870	1HG2 VAL A 575	-13.305	-5.960	-12.463	1.00	0.00
ATOM	871	2HG2 VAL A 575	-14.897	-6.619	-12.089	1.00	0.00
ATOM	872	3HG2 VAL A 575	-13.459	-7.670	-12.059	1.00	0.00
ATOM	873	N LYS A 576	-16.162	-4.895	-9.209	1.00	0.00
ATOM	874	CA LYS A 576	-17.590	-4.759	-9.248	1.00	0.00
ATOM	875	C LYS A 576	-17.917	-3.345	-9.608	1.00	0.00
ATOM	876	O LYS A 576	-18.759	-3.086	-10.468	1.00	0.00
ATOM	877	CB LYS A 576	-18.241	-4.998	-7.873	1.00	0.00
ATOM	878	CG LYS A 576	-17.958	-6.373	-7.268	1.00	0.00
ATOM	879	CD LYS A 576	-18.478	-7.544	-8.101	1.00	0.00
ATOM	880	CE LYS A 576	-18.182	-8.907	-7.472	1.00	0.00
ATOM	881	NZ LYS A 576	-18.714	-9.988	-8.331	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

34/208

ATOM	882	HN	LYS A 576	-15.722	-5.152	-8.349	1.00	0.00
ATOM	883	HA	LYS A 576	-17.956	-5.490	-9.969	1.00	0.00
ATOM	884	1HB	LYS A 576	-19.319	-4.882	-7.977	1.00	0.00
ATOM	885	2HB	LYS A 576	-17.879	-4.236	-7.184	1.00	0.00
ATOM	886	1HG	LYS A 576	-18.419	-6.419	-6.282	1.00	0.00
ATOM	887	2HG	LYS A 576	-16.881	-6.484	-7.149	1.00	0.00
ATOM	888	1HD	LYS A 576	-18.017	-7.506	-9.088	1.00	0.00
ATOM	889	2HD	LYS A 576	-19.555	-7.439	-8.222	1.00	0.00
ATOM	890	1HE	LYS A 576	-18.657	-8.984	-6.494	1.00	0.00
ATOM	891	2HE	LYS A 576	-17.107	-9.052	-7.369	1.00	0.00
ATOM	892	1HZ	LYS A 576	-18.266	-9.940	-9.267	1.00	0.00
ATOM	893	2HZ	LYS A 576	-19.743	-9.875	-8.433	1.00	0.00
ATOM	894	3HZ	LYS A 576	-18.509	-10.910	-7.895	1.00	0.00
ATOM	895	N	TRP A 577	-17.222	-2.390	-8.964	1.00	0.00
ATOM	896	CA	TRP A 577	-17.460	-0.991	-9.166	1.00	0.00
ATOM	897	C	TRP A 577	-17.218	-0.636	-10.591	1.00	0.00
ATOM	898	O	TRP A 577	-17.991	0.096	-11.206	1.00	0.00
ATOM	899	CB	TRP A 577	-16.491	-0.113	-8.355	1.00	0.00
ATOM	900	CG	TRP A 577	-16.575	1.365	-8.665	1.00	0.00
ATOM	901	CD1	TRP A 577	-17.346	2.331	-8.087	1.00	0.00
ATOM	902	CD2	TRP A 577	-15.783	2.025	-9.667	1.00	0.00
ATOM	903	NE1	TRP A 577	-17.099	3.546	-8.679	1.00	0.00
ATOM	904	CE2	TRP A 577	-16.136	3.374	-9.651	1.00	0.00
ATOM	905	CE3	TRP A 577	-14.836	1.549	-10.529	1.00	0.00
ATOM	906	CZ2	TRP A 577	-15.548	4.269	-10.500	1.00	0.00
ATOM	907	CZ3	TRP A 577	-14.245	2.455	-11.383	1.00	0.00
ATOM	908	CH2	TRP A 577	-14.593	3.789	-11.370	1.00	0.00
ATOM	909	HN	TRP A 577	-16.511	-2.669	-8.319	1.00	0.00
ATOM	910	HA	TRP A 577	-18.489	-0.799	-8.860	1.00	0.00
ATOM	911	1HB	TRP A 577	-15.471	-0.439	-8.555	1.00	0.00
ATOM	912	2HB	TRP A 577	-16.703	-0.245	-7.294	1.00	0.00
ATOM	913	HE3	TRP A 577	-14.563	0.505	-10.542	1.00	0.00
ATOM	914	HD1	TRP A 577	-18.047	2.165	-7.283	1.00	0.00
ATOM	915	HE1	TRP A 577	-17.534	4.393	-8.450	1.00	0.00
ATOM	916	HZ2	TRP A 577	-15.821	5.314	-10.490	1.00	0.00
ATOM	917	HZ3	TRP A 577	-13.492	2.113	-12.077	1.00	0.00
ATOM	918	HH2	TRP A 577	-14.109	4.470	-12.054	1.00	0.00
ATOM	919	N	ALA A 578	-16.141	-1.186	-11.164	1.00	0.00
ATOM	920	CA	ALA A 578	-15.751	-0.831	-12.495	1.00	0.00
ATOM	921	C	ALA A 578	-16.858	-1.134	-13.453	1.00	0.00
ATOM	922	O	ALA A 578	-17.130	-0.350	-14.361	1.00	0.00
ATOM	923	CB	ALA A 578	-14.504	-1.599	-12.969	1.00	0.00
ATOM	924	HN	ALA A 578	-15.601	-1.856	-10.654	1.00	0.00
ATOM	925	HA	ALA A 578	-15.554	0.240	-12.488	1.00	0.00
ATOM	926	1HB	ALA A 578	-14.737	-2.651	-13.130	1.00	0.00
ATOM	927	2HB	ALA A 578	-13.717	-1.539	-12.217	1.00	0.00
ATOM	928	3HB	ALA A 578	-14.143	-1.185	-13.910	1.00	0.00
ATOM	929	N	LYS A 579	-17.560	-2.259	-13.246	1.00	0.00
ATOM	930	CA	LYS A 579	-18.569	-2.685	-14.173	1.00	0.00

35/208

ATOM	931	C	LYS A 579	-19.602	-1.613	-14.317	1.00	0.00
ATOM	932	O	LYS A 579	-20.149	-1.402	-15.396	1.00	0.00
ATOM	933	CB	LYS A 579	-19.301	-3.950	-13.690	1.00	0.00
ATOM	934	CG	LYS A 579	-18.376	-5.153	-13.491	1.00	0.00
ATOM	935	CD	LYS A 579	-17.692	-5.639	-14.770	1.00	0.00
ATOM	936	CE	LYS A 579	-18.527	-6.650	-15.559	1.00	0.00
ATOM	937	NZ	LYS A 579	-17.774	-7.115	-16.747	1.00	0.00
ATOM	938	HN	LYS A 579	-17.377	-2.809	-12.431	1.00	0.00
ATOM	939	HA	LYS A 579	-18.066	-2.878	-15.120	1.00	0.00
ATOM	940	1HB	LYS A 579	-20.064	-4.212	-14.421	1.00	0.00
ATOM	941	2HB	LYS A 579	-19.795	-3.728	-12.745	1.00	0.00
ATOM	942	1HG	LYS A 579	-18.961	-5.974	-13.079	1.00	0.00
ATOM	943	2HG	LYS A 579	-17.608	-4.882	-12.769	1.00	0.00
ATOM	944	1HD	LYS A 579	-16.742	-6.101	-14.505	1.00	0.00
ATOM	945	2HD	LYS A 579	-17.489	-4.779	-15.407	1.00	0.00
ATOM	946	1HE	LYS A 579	-19.454	-6.190	-15.903	1.00	0.00
ATOM	947	2HE	LYS A 579	-18.756	-7.518	-14.941	1.00	0.00
ATOM	948	1HZ	LYS A 579	-17.214	-7.954	-16.495	1.00	0.00
ATOM	949	2HZ	LYS A 579	-17.139	-6.358	-17.072	1.00	0.00
ATOM	950	3HZ	LYS A 579	-18.441	-7.358	-17.507	1.00	0.00
ATOM	951	N	ALA A 580	-19.912	-0.937	-13.203	1.00	0.00
ATOM	952	CA	ALA A 580	-20.909	0.087	-13.093	1.00	0.00
ATOM	953	C	ALA A 580	-20.599	1.416	-13.730	1.00	0.00
ATOM	954	O	ALA A 580	-21.517	2.183	-14.014	1.00	0.00
ATOM	955	CB	ALA A 580	-21.275	0.329	-11.631	1.00	0.00
ATOM	956	HN	ALA A 580	-19.401	-1.166	-12.376	1.00	0.00
ATOM	957	HA	ALA A 580	-21.779	-0.250	-13.656	1.00	0.00
ATOM	958	1HB	ALA A 580	-20.701	-0.327	-10.976	1.00	0.00
ATOM	959	2HB	ALA A 580	-22.333	0.125	-11.469	1.00	0.00
ATOM	960	3HB	ALA A 580	-21.054	1.359	-11.353	1.00	0.00
ATOM	961	N	ILE A 581	-19.308	1.770	-13.915	1.00	0.00
ATOM	962	CA	ILE A 581	-19.009	3.067	-14.463	1.00	0.00
ATOM	963	C	ILE A 581	-19.485	3.141	-15.877	1.00	0.00
ATOM	964	O	ILE A 581	-19.052	2.378	-16.741	1.00	0.00
ATOM	965	CB	ILE A 581	-17.545	3.400	-14.445	1.00	0.00
ATOM	966	CG1	ILE A 581	-17.304	4.796	-15.038	1.00	0.00
ATOM	967	CG2	ILE A 581	-16.779	2.273	-15.149	1.00	0.00
ATOM	968	CD1	ILE A 581	-15.857	5.261	-14.898	1.00	0.00
ATOM	969	HN	ILE A 581	-18.571	1.139	-13.674	1.00	0.00
ATOM	970	HA	ILE A 581	-19.563	3.791	-13.865	1.00	0.00
ATOM	971	HB	ILE A 581	-17.198	3.501	-13.417	1.00	0.00
ATOM	972	1HG2	ILE A 581	-17.468	1.591	-15.648	1.00	0.00
ATOM	973	2HG2	ILE A 581	-16.203	1.699	-14.424	1.00	0.00
ATOM	974	3HG2	ILE A 581	-16.110	2.687	-15.903	1.00	0.00
ATOM	975	1HG1	ILE A 581	-17.954	5.510	-14.534	1.00	0.00
ATOM	976	2HG1	ILE A 581	-17.568	4.780	-16.095	1.00	0.00
ATOM	977	1HD1	ILE A 581	-15.168	4.438	-15.083	1.00	0.00
ATOM	978	2HD1	ILE A 581	-15.677	5.630	-13.888	1.00	0.00
ATOM	979	3HD1	ILE A 581	-15.643	6.049	-15.620	1.00	0.00

36/208

ATOM	980	N	PRO A 582	-20.368	4.076	-16.116	1.00	0.00
ATOM	981	CA	PRO A 582	-20.989	4.240	-17.404	1.00	0.00
ATOM	982	C	PRO A 582	-19.969	4.258	-18.500	1.00	0.00
ATOM	983	O	PRO A 582	-19.001	5.010	-18.407	1.00	0.00
ATOM	984	CB	PRO A 582	-21.759	5.557	-17.322	1.00	0.00
ATOM	985	CG	PRO A 582	-20.958	6.369	-16.287	1.00	0.00
ATOM	986	CD	PRO A 582	-20.393	5.302	-15.335	1.00	0.00
ATOM	987	IHD	PRO A 582	-19.386	5.561	-15.006	1.00	0.00
ATOM	988	2HD	PRO A 582	-21.029	5.179	-14.458	1.00	0.00
ATOM	989	HA	PRO A 582	-21.661	3.406	-17.606	1.00	0.00
ATOM	990	IHB	PRO A 582	-22.786	5.397	-16.993	1.00	0.00
ATOM	991	2HB	PRO A 582	-21.785	6.062	-18.287	1.00	0.00
ATOM	992	IHG	PRO A 582	-20.158	6.934	-16.764	1.00	0.00
ATOM	993	2HG	PRO A 582	-21.601	7.070	-15.754	1.00	0.00
ATOM	994	N	GLY A 583	-20.176	3.417	-19.535	1.00	0.00
ATOM	995	CA	GLY A 583	-19.319	3.366	-20.683	1.00	0.00
ATOM	996	C	GLY A 583	-18.265	2.305	-20.568	1.00	0.00
ATOM	997	O	GLY A 583	-17.716	1.855	-21.571	1.00	0.00
ATOM	998	HN	GLY A 583	-20.964	2.802	-19.498	1.00	0.00
ATOM	999	IHA	GLY A 583	-18.842	4.341	-20.773	1.00	0.00
ATOM	1000	2HA	GLY A 583	-19.950	3.155	-21.547	1.00	0.00
ATOM	1001	N	PHE A 584	-17.960	1.858	-19.339	1.00	0.00
ATOM	1002	CA	PHE A 584	-16.904	0.905	-19.124	1.00	0.00
ATOM	1003	C	PHE A 584	-17.199	-0.427	-19.753	1.00	0.00
ATOM	1004	O	PHE A 584	-16.348	-1.026	-20.411	1.00	0.00
ATOM	1005	CB	PHE A 584	-16.664	0.684	-17.623	1.00	0.00
ATOM	1006	CG	PHE A 584	-15.471	-0.178	-17.407	1.00	0.00
ATOM	1007	CD1	PHE A 584	-14.204	0.322	-17.608	1.00	0.00
ATOM	1008	CD2	PHE A 584	-15.612	-1.384	-16.760	1.00	0.00
ATOM	1009	CE1	PHE A 584	-13.096	-0.406	-17.241	1.00	0.00
ATOM	1010	CE2	PHE A 584	-14.509	-2.100	-16.364	1.00	0.00
ATOM	1011	CZ	PHE A 584	-13.246	-1.619	-16.614	1.00	0.00
ATOM	1012	HN	PHE A 584	-18.479	2.197	-18.555	1.00	0.00
ATOM	1013	HA	PHE A 584	-16.008	1.303	-19.601	1.00	0.00
ATOM	1014	IHB	PHE A 584	-17.533	0.202	-17.177	1.00	0.00
ATOM	1015	2HB	PHE A 584	-16.501	1.643	-17.131	1.00	0.00
ATOM	1016	HD1	PHE A 584	-14.079	1.296	-18.058	1.00	0.00
ATOM	1017	HD2	PHE A 584	-16.600	-1.771	-16.561	1.00	0.00
ATOM	1018	HE1	PHE A 584	-12.107	-0.023	-17.446	1.00	0.00
ATOM	1019	HE2	PHE A 584	-14.635	-3.044	-15.854	1.00	0.00
ATOM	1020	HZ	PHE A 584	-12.378	-2.190	-16.320	1.00	0.00
ATOM	1021	N	ARG A 585	-18.450	-0.893	-19.595	1.00	0.00
ATOM	1022	CA	ARG A 585	-18.881	-2.187	-20.037	1.00	0.00
ATOM	1023	C	ARG A 585	-18.770	-2.297	-21.522	1.00	0.00
ATOM	1024	O	ARG A 585	-18.582	-3.387	-22.060	1.00	0.00
ATOM	1025	CB	ARG A 585	-20.341	-2.478	-19.653	1.00	0.00
ATOM	1026	CG	ARG A 585	-20.830	-3.866	-20.073	1.00	0.00
ATOM	1027	CD	ARG A 585	-22.284	-4.140	-19.683	1.00	0.00
ATOM	1028	NE	ARG A 585	-22.624	-5.515	-20.148	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

37/208

ATOM	1029	CZ	ARG A 585	-23.782	-6.107	-19.736	1.00	0.00
ATOM	1030	NH1	ARG A 585	-24.095	-7.365	-20.161	1.00	0.00
ATOM	1031	NH2	ARG A 585	-24.629	-5.440	-18.897	1.00	0.00
ATOM	1032	HN	ARG A 585	-19.118	-0.302	-19.143	1.00	0.00
ATOM	1033	HA	ARG A 585	-18.217	-2.916	-19.573	1.00	0.00
ATOM	1034	1HB	ARG A 585	-20.979	-1.730	-20.120	1.00	0.00
ATOM	1035	2HB	ARG A 585	-20.441	-2.387	-18.572	1.00	0.00
ATOM	1036	1HG	ARG A 585	-20.194	-4.617	-19.605	1.00	0.00
ATOM	1037	2HG	ARG A 585	-20.732	-3.959	-21.154	1.00	0.00
ATOM	1038	1HD	ARG A 585	-22.963	-3.442	-20.172	1.00	0.00
ATOM	1039	2HD	ARG A 585	-22.418	-4.107	-18.603	1.00	0.00
ATOM	1040	HE	ARG A 585	-22.003	-6.004	-20.760	1.00	0.00
ATOM	1041	1HH1	ARG A 585	-23.475	-7.854	-20.775	1.00	0.00
ATOM	1042	2HH1	ARG A 585	-24.944	-7.798	-19.860	1.00	0.00
ATOM	1043	1HH2	ARG A 585	-24.480	-4.471	-18.703	1.00	0.00
ATOM	1044	2HH2	ARG A 585	-25.398	-5.922	-18.477	1.00	0.00
ATOM	1045	N	ASN A 586	-18.893	-1.162	-22.227	1.00	0.00
ATOM	1046	CA	ASN A 586	-18.871	-1.149	-23.658	1.00	0.00
ATOM	1047	C	ASN A 586	-17.577	-1.675	-24.203	1.00	0.00
ATOM	1048	O	ASN A 586	-17.544	-2.196	-25.315	1.00	0.00
ATOM	1049	CB	ASN A 586	-19.118	0.251	-24.236	1.00	0.00
ATOM	1050	CG	ASN A 586	-20.571	0.587	-23.938	1.00	0.00
ATOM	1051	OD1	ASN A 586	-21.465	-0.218	-24.195	1.00	0.00
ATOM	1052	ND2	ASN A 586	-20.815	1.795	-23.364	1.00	0.00
ATOM	1053	HN	ASN A 586	-19.004	-0.298	-21.736	1.00	0.00
ATOM	1054	HA	ASN A 586	-19.650	-1.836	-23.990	1.00	0.00
ATOM	1055	1HB	ASN A 586	-18.950	0.263	-25.312	1.00	0.00
ATOM	1056	2HB	ASN A 586	-18.466	0.987	-23.765	1.00	0.00
ATOM	1057	1HD2	ASN A 586	-20.132	2.522	-23.430	1.00	0.00
ATOM	1058	2HD2	ASN A 586	-21.669	1.973	-22.876	1.00	0.00
ATOM	1059	N	LEU A 587	-16.462	-1.528	-23.464	1.00	0.00
ATOM	1060	CA	LEU A 587	-15.216	-2.041	-23.971	1.00	0.00
ATOM	1061	C	LEU A 587	-15.207	-3.534	-23.839	1.00	0.00
ATOM	1062	O	LEU A 587	-15.985	-4.117	-23.087	1.00	0.00
ATOM	1063	CB	LEU A 587	-13.966	-1.549	-23.218	1.00	0.00
ATOM	1064	CG	LEU A 587	-13.683	-0.036	-23.312	1.00	0.00
ATOM	1065	CD1	LEU A 587	-14.647	0.804	-22.461	1.00	0.00
ATOM	1066	CD2	LEU A 587	-12.217	0.255	-22.978	1.00	0.00
ATOM	1067	HN	LEU A 587	-16.499	-1.069	-22.577	1.00	0.00
ATOM	1068	HA	LEU A 587	-15.162	-1.731	-25.014	1.00	0.00
ATOM	1069	1HB	LEU A 587	-13.102	-2.081	-23.612	1.00	0.00
ATOM	1070	2HB	LEU A 587	-14.080	-1.809	-22.167	1.00	0.00
ATOM	1071	HG	LEU A 587	-13.768	0.275	-24.352	1.00	0.00
ATOM	1072	1HD1	LEU A 587	-14.703	0.414	-21.445	1.00	0.00
ATOM	1073	2HD1	LEU A 587	-15.649	0.776	-22.889	1.00	0.00
ATOM	1074	3HD1	LEU A 587	-14.300	1.836	-22.407	1.00	0.00
ATOM	1075	1HD2	LEU A 587	-11.554	-0.262	-23.671	1.00	0.00
ATOM	1076	2HD2	LEU A 587	-11.985	-0.088	-21.970	1.00	0.00
ATOM	1077	3HD2	LEU A 587	-12.019	1.324	-23.056	1.00	0.00

38/208

ATOM	1078	N	HIS A 588	-14.324	-4.224	-24.583	1.00	0.00
ATOM	1079	CA	HIS A 588	-14.302	-5.645	-24.394	1.00	0.00
ATOM	1080	C	HIS A 588	-13.680	-5.962	-23.057	1.00	0.00
ATOM	1081	O	HIS A 588	-13.397	-5.069	-22.263	1.00	0.00
ATOM	1082	CB	HIS A 588	-13.564	-6.456	-25.471	1.00	0.00
ATOM	1083	CG	HIS A 588	-14.329	-6.632	-26.751	1.00	0.00
ATOM	1084	ND1	HIS A 588	-14.228	-5.801	-27.843	1.00	0.00
ATOM	1085	CD2	HIS A 588	-15.196	-7.619	-27.114	1.00	0.00
ATOM	1086	CE1	HIS A 588	-15.033	-6.320	-28.805	1.00	0.00
ATOM	1087	NE2	HIS A 588	-15.641	-7.422	-28.409	1.00	0.00
ATOM	1088	HN	HIS A 588	-13.715	-3.769	-25.232	1.00	0.00
ATOM	1089	HA	HIS A 588	-15.346	-5.955	-24.360	1.00	0.00
ATOM	1090	1HB	HIS A 588	-13.344	-7.446	-25.075	1.00	0.00
ATOM	1091	2HB	HIS A 588	-12.627	-5.953	-25.708	1.00	0.00
ATOM	1092	HD2	HIS A 588	-15.494	-8.439	-26.479	1.00	0.00
ATOM	1093	HD1	HIS A 588	-13.681	-4.992	-27.913	1.00	0.00
ATOM	1094	HE1	HIS A 588	-15.160	-5.881	-29.783	1.00	0.00
ATOM	1095	N	LEU A 589	-13.524	-7.268	-22.754	1.00	0.00
ATOM	1096	CA	LEU A 589	-12.907	-7.782	-21.549	1.00	0.00
ATOM	1097	C	LEU A 589	-11.421	-7.545	-21.600	1.00	0.00
ATOM	1098	O	LEU A 589	-10.690	-7.638	-20.621	1.00	0.00
ATOM	1099	CB	LEU A 589	-13.182	-9.270	-21.281	1.00	0.00
ATOM	1100	CG	LEU A 589	-14.650	-9.519	-20.885	1.00	0.00
ATOM	1101	CD1	LEU A 589	-15.603	-9.313	-22.073	1.00	0.00
ATOM	1102	CD2	LEU A 589	-14.825	-10.869	-20.181	1.00	0.00
ATOM	1103	HN	LEU A 589	-13.862	-7.935	-23.416	1.00	0.00
ATOM	1104	HA	LEU A 589	-13.296	-7.182	-20.728	1.00	0.00
ATOM	1105	1HB	LEU A 589	-12.532	-9.615	-20.478	1.00	0.00
ATOM	1106	2HB	LEU A 589	-12.952	-9.844	-22.178	1.00	0.00
ATOM	1107	HG	LEU A 589	-14.925	-8.835	-20.083	1.00	0.00
ATOM	1108	1HD1	LEU A 589	-15.171	-9.716	-22.989	1.00	0.00
ATOM	1109	2HD1	LEU A 589	-15.789	-8.250	-22.227	1.00	0.00
ATOM	1110	3HD1	LEU A 589	-16.547	-9.827	-21.892	1.00	0.00
ATOM	1111	1HD2	LEU A 589	-14.225	-10.909	-19.272	1.00	0.00
ATOM	1112	2HD2	LEU A 589	-14.502	-11.679	-20.834	1.00	0.00
ATOM	1113	3HD2	LEU A 589	-15.868	-11.016	-19.902	1.00	0.00
ATOM	1114	N	ASP A 590	-11.031	-7.149	-22.805	1.00	0.00
ATOM	1115	CA	ASP A 590	-9.924	-6.818	-23.641	1.00	0.00
ATOM	1116	C	ASP A 590	-10.032	-5.373	-23.370	1.00	0.00
ATOM	1117	O	ASP A 590	-11.115	-4.836	-23.268	1.00	0.00
ATOM	1118	CB	ASP A 590	-10.004	-7.103	-25.178	1.00	0.00
ATOM	1119	CG	ASP A 590	-10.722	-6.130	-26.144	1.00	0.00
ATOM	1120	OD1	ASP A 590	-10.727	-6.510	-27.345	1.00	0.00
ATOM	1121	OD2	ASP A 590	-11.240	-5.041	-25.780	1.00	0.00
ATOM	1122	HN	ASP A 590	-11.837	-7.036	-23.342	1.00	0.00
ATOM	1123	HA	ASP A 590	-9.087	-7.380	-23.229	1.00	0.00
ATOM	1124	1HB	ASP A 590	-10.503	-8.061	-25.301	1.00	0.00
ATOM	1125	2HB	ASP A 590	-8.982	-7.178	-25.542	1.00	0.00
ATOM	1126	N	ASP A 591	-8.993	-4.639	-23.046	1.00	0.00



39/208

ATOM	1127	CA	ASP A 591	-8.947	-3.488	-22.220	1.00	0.00
ATOM	1128	C	ASP A 591	-9.839	-3.337	-21.017	1.00	0.00
ATOM	1129	O	ASP A 591	-9.322	-2.693	-20.111	1.00	0.00
ATOM	1130	CB	ASP A 591	-9.244	-2.289	-23.151	1.00	0.00
ATOM	1131	CG	ASP A 591	-9.012	-0.909	-22.554	1.00	0.00
ATOM	1132	OD1	ASP A 591	-8.376	-0.782	-21.477	1.00	0.00
ATOM	1133	OD2	ASP A 591	-9.478	0.062	-23.206	1.00	0.00
ATOM	1134	HN	ASP A 591	-8.121	-4.930	-23.433	1.00	0.00
ATOM	1135	HA	ASP A 591	-7.953	-3.420	-21.779	1.00	0.00
ATOM	1136	IHB	ASP A 591	-10.289	-2.337	-23.455	1.00	0.00
ATOM	1137	2HB	ASP A 591	-8.611	-2.370	-24.034	1.00	0.00
ATOM	1138	N	GLN A 592	-11.100	-3.786	-20.880	1.00	0.00
ATOM	1139	CA	GLN A 592	-11.706	-3.638	-19.564	1.00	0.00
ATOM	1140	C	GLN A 592	-10.809	-4.237	-18.494	1.00	0.00
ATOM	1141	O	GLN A 592	-10.526	-3.611	-17.468	1.00	0.00
ATOM	1142	CB	GLN A 592	-13.062	-4.362	-19.519	1.00	0.00
ATOM	1143	CG	GLN A 592	-13.773	-4.302	-18.176	1.00	0.00
ATOM	1144	CD	GLN A 592	-15.098	-5.034	-18.326	1.00	0.00
ATOM	1145	OE1	GLN A 592	-15.704	-5.451	-17.341	1.00	0.00
ATOM	1146	NE2	GLN A 592	-15.565	-5.192	-19.595	1.00	0.00
ATOM	1147	HN	GLN A 592	-11.595	-4.199	-21.643	1.00	0.00
ATOM	1148	HA	GLN A 592	-11.832	-2.572	-19.381	1.00	0.00
ATOM	1149	IHB	GLN A 592	-12.902	-5.408	-19.776	1.00	0.00
ATOM	1150	2HB	GLN A 592	-13.713	-3.919	-20.272	1.00	0.00
ATOM	1151	IHG	GLN A 592	-13.961	-3.268	-17.886	1.00	0.00
ATOM	1152	2HG	GLN A 592	-13.177	-4.786	-17.402	1.00	0.00
ATOM	1153	IHE2	GLN A 592	-15.039	-4.833	-20.365	1.00	0.00
ATOM	1154	2HE2	GLN A 592	-16.429	-5.663	-19.774	1.00	0.00
ATOM	1155	N	MET A 593	-10.260	-5.437	-18.742	1.00	0.00
ATOM	1156	CA	MET A 593	-9.370	-6.015	-17.780	1.00	0.00
ATOM	1157	C	MET A 593	-8.169	-5.123	-17.698	1.00	0.00
ATOM	1158	O	MET A 593	-7.646	-4.868	-16.610	1.00	0.00
ATOM	1159	CB	MET A 593	-8.929	-7.431	-18.199	1.00	0.00
ATOM	1160	CG	MET A 593	-8.478	-8.331	-17.047	1.00	0.00
ATOM	1161	SD	MET A 593	-6.901	-7.880	-16.276	1.00	0.00
ATOM	1162	CE	MET A 593	-6.846	-9.316	-15.164	1.00	0.00
ATOM	1163	HN	MET A 593	-10.471	-5.922	-19.591	1.00	0.00
ATOM	1164	HA	MET A 593	-9.905	-6.049	-16.831	1.00	0.00
ATOM	1165	IHB	MET A 593	-8.104	-7.338	-18.905	1.00	0.00
ATOM	1166	2HB	MET A 593	-9.762	-7.914	-18.707	1.00	0.00
ATOM	1167	IHG	MET A 593	-8.383	-9.350	-17.420	1.00	0.00
ATOM	1168	2HG	MET A 593	-9.242	-8.309	-16.271	1.00	0.00
ATOM	1169	IHE	MET A 593	-6.846	-10.232	-15.754	1.00	0.00
ATOM	1170	2HE	MET A 593	-7.723	-9.318	-14.517	1.00	0.00
ATOM	1171	3HE	MET A 593	-5.935	-9.286	-14.566	1.00	0.00
ATOM	1172	N	THR A 594	-7.699	-4.597	-18.851	1.00	0.00
ATOM	1173	CA	THR A 594	-6.500	-3.820	-18.739	1.00	0.00
ATOM	1174	C	THR A 594	-6.684	-2.533	-17.985	1.00	0.00
ATOM	1175	O	THR A 594	-5.791	-2.161	-17.226	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

40/208

ATOM	1176	CB	THR A 594	-5.721	-3.609	-20.009	1.00	0.00
ATOM	1177	OG1	THR A 594	-4.434	-3.097	-19.695	1.00	0.00
ATOM	1178	CG2	THR A 594	-6.449	-2.635	-20.928	1.00	0.00
ATOM	1179	HN	THR A 594	-8.159	-4.741	-19.727	1.00	0.00
ATOM	1180	HA	THR A 594	-5.875	-4.345	-18.016	1.00	0.00
ATOM	1181	HB	THR A 594	-5.596	-4.552	-20.541	1.00	0.00
ATOM	1182	HG1	THR A 594	-4.553	-2.470	-18.995	1.00	0.00
ATOM	1183	1HG2	THR A 594	-5.913	-1.688	-20.989	1.00	0.00
ATOM	1184	2HG2	THR A 594	-7.449	-2.432	-20.545	1.00	0.00
ATOM	1185	3HG2	THR A 594	-6.519	-3.048	-21.935	1.00	0.00
ATOM	1186	N	LEU A 595	-7.840	-1.833	-18.125	1.00	0.00
ATOM	1187	CA	LEU A 595	-7.992	-0.587	-17.402	1.00	0.00
ATOM	1188	C	LEU A 595	-7.869	-0.929	-15.955	1.00	0.00
ATOM	1189	O	LEU A 595	-7.238	-0.225	-15.165	1.00	0.00
ATOM	1190	CB	LEU A 595	-9.378	0.113	-17.468	1.00	0.00
ATOM	1191	CG	LEU A 595	-9.880	0.767	-18.781	1.00	0.00
ATOM	1192	CD1	LEU A 595	-8.871	1.762	-19.367	1.00	0.00
ATOM	1193	CD2	LEU A 595	-10.458	-0.238	-19.780	1.00	0.00
ATOM	1194	HN	LEU A 595	-8.572	-2.172	-18.715	1.00	0.00
ATOM	1195	HA	LEU A 595	-7.237	0.081	-17.815	1.00	0.00
ATOM	1196	1HB	LEU A 595	-9.370	0.895	-16.713	1.00	0.00
ATOM	1197	2HB	LEU A 595	-10.118	-0.633	-17.189	1.00	0.00
ATOM	1198	HG	LEU A 595	-10.816	1.288	-18.582	1.00	0.00
ATOM	1199	1HD1	LEU A 595	-7.996	1.240	-19.756	1.00	0.00
ATOM	1200	2HD1	LEU A 595	-8.534	2.455	-18.596	1.00	0.00
ATOM	1201	3HD1	LEU A 595	-9.323	2.318	-20.188	1.00	0.00
ATOM	1202	1HD2	LEU A 595	-11.538	-0.117	-19.866	1.00	0.00
ATOM	1203	2HD2	LEU A 595	-10.259	-1.257	-19.447	1.00	0.00
ATOM	1204	3HD2	LEU A 595	-10.022	-0.082	-20.766	1.00	0.00
ATOM	1205	N	LEU A 596	-8.477	-2.053	-15.561	1.00	0.00
ATOM	1206	CA	LEU A 596	-8.431	-2.348	-14.173	1.00	0.00
ATOM	1207	C	LEU A 596	-7.005	-2.577	-13.776	1.00	0.00
ATOM	1208	O	LEU A 596	-6.529	-2.006	-12.796	1.00	0.00
ATOM	1209	CB	LEU A 596	-9.288	-3.570	-13.814	1.00	0.00
ATOM	1210	CG	LEU A 596	-9.576	-3.691	-12.312	1.00	0.00
ATOM	1211	CD1	LEU A 596	-10.386	-2.487	-11.801	1.00	0.00
ATOM	1212	CD2	LEU A 596	-10.268	-5.021	-11.996	1.00	0.00
ATOM	1213	HN	LEU A 596	-8.941	-2.654	-16.211	1.00	0.00
ATOM	1214	HA	LEU A 596	-8.795	-1.465	-13.649	1.00	0.00
ATOM	1215	1HB	LEU A 596	-8.772	-4.470	-14.146	1.00	0.00
ATOM	1216	2HB	LEU A 596	-10.235	-3.502	-14.348	1.00	0.00
ATOM	1217	HG	LEU A 596	-8.634	-3.749	-11.768	1.00	0.00
ATOM	1218	1HD1	LEU A 596	-11.255	-2.310	-12.434	1.00	0.00
ATOM	1219	2HD1	LEU A 596	-9.771	-1.587	-11.813	1.00	0.00
ATOM	1220	3HD1	LEU A 596	-10.740	-2.674	-10.787	1.00	0.00
ATOM	1221	1HD2	LEU A 596	-9.639	-5.862	-12.290	1.00	0.00
ATOM	1222	2HD2	LEU A 596	-11.208	-5.096	-12.542	1.00	0.00
ATOM	1223	3HD2	LEU A 596	-10.459	-5.102	-10.926	1.00	0.00
ATOM	1224	N	GLN A 597	-6.254	-3.356	-14.577	1.00	0.00

41/208

ATOM	1225	CA	GLN A 597	-4.895	-3.650	-14.216	1.00	0.00
ATOM	1226	C	GLN A 597	-4.138	-2.371	-14.131	1.00	0.00
ATOM	1227	O	GLN A 597	-3.312	-2.175	-13.242	1.00	0.00
ATOM	1228	CB	GLN A 597	-4.169	-4.488	-15.273	1.00	0.00
ATOM	1229	CG	GLN A 597	-4.725	-5.897	-15.424	1.00	0.00
ATOM	1230	CD	GLN A 597	-3.981	-6.553	-16.577	1.00	0.00
ATOM	1231	OE1	GLN A 597	-3.425	-7.638	-16.436	1.00	0.00
ATOM	1232	NE2	GLN A 597	-3.972	-5.874	-17.757	1.00	0.00
ATOM	1233	HN	GLN A 597	-6.641	-3.728	-15.421	1.00	0.00
ATOM	1234	HA	GLN A 597	-4.932	-4.189	-13.270	1.00	0.00
ATOM	1235	1HB	GLN A 597	-3.117	-4.556	-15.001	1.00	0.00
ATOM	1236	2HB	GLN A 597	-4.243	-3.979	-16.233	1.00	0.00
ATOM	1237	1HG	GLN A 597	-5.791	-5.870	-15.647	1.00	0.00
ATOM	1238	2HG	GLN A 597	-4.566	-6.474	-14.513	1.00	0.00
ATOM	1239	1HE2	GLN A 597	-4.441	-4.994	-17.826	1.00	0.00
ATOM	1240	2HE2	GLN A 597	-3.505	-6.240	-18.561	1.00	0.00
ATOM	1241	N	TYR A 598	-4.409	-1.463	-15.078	1.00	0.00
ATOM	1242	CA	TYR A 598	-3.683	-0.231	-15.173	1.00	0.00
ATOM	1243	C	TYR A 598	-3.830	0.698	-14.007	1.00	0.00
ATOM	1244	O	TYR A 598	-2.830	1.205	-13.499	1.00	0.00
ATOM	1245	CB	TYR A 598	-4.094	0.568	-16.422	1.00	0.00
ATOM	1246	CG	TYR A 598	-3.326	1.843	-16.414	1.00	0.00
ATOM	1247	CD1	TYR A 598	-2.013	1.869	-16.821	1.00	0.00
ATOM	1248	CD2	TYR A 598	-3.932	3.021	-16.038	1.00	0.00
ATOM	1249	CE1	TYR A 598	-1.307	3.047	-16.831	1.00	0.00
ATOM	1250	CE2	TYR A 598	-3.231	4.204	-16.048	1.00	0.00
ATOM	1251	CZ	TYR A 598	-1.914	4.216	-16.440	1.00	0.00
ATOM	1252	OH	TYR A 598	-1.187	5.426	-16.448	1.00	0.00
ATOM	1253	HN	TYR A 598	-5.138	-1.650	-15.736	1.00	0.00
ATOM	1254	HA	TYR A 598	-2.624	-0.488	-15.217	1.00	0.00
ATOM	1255	1HB	TYR A 598	-5.162	0.784	-16.403	1.00	0.00
ATOM	1256	2HB	TYR A 598	-3.864	0.008	-17.328	1.00	0.00
ATOM	1257	HD1	TYR A 598	-1.532	0.954	-17.137	1.00	0.00
ATOM	1258	HE1	TYR A 598	-0.274	3.055	-17.146	1.00	0.00
ATOM	1259	HD2	TYR A 598	-4.968	3.015	-15.733	1.00	0.00
ATOM	1260	HE2	TYR A 598	-3.715	5.122	-15.749	1.00	0.00
ATOM	1261	HH	TYR A 598	-1.413	5.935	-15.680	1.00	0.00
ATOM	1262	N	SER A 599	-5.066	0.937	-13.524	1.00	0.00
ATOM	1263	CA	SER A 599	-5.201	1.987	-12.548	1.00	0.00
ATOM	1264	C	SER A 599	-5.623	1.487	-11.203	1.00	0.00
ATOM	1265	O	SER A 599	-6.170	2.237	-10.397	1.00	0.00
ATOM	1266	CB	SER A 599	-6.228	3.049	-13.002	1.00	0.00
ATOM	1267	OG	SER A 599	-6.261	4.154	-12.109	1.00	0.00
ATOM	1268	HN	SER A 599	-5.856	0.407	-13.831	1.00	0.00
ATOM	1269	HA	SER A 599	-4.216	2.438	-12.425	1.00	0.00
ATOM	1270	1HB	SER A 599	-7.227	2.613	-13.032	1.00	0.00
ATOM	1271	2HB	SER A 599	-5.964	3.424	-13.991	1.00	0.00
ATOM	1272	HG	SER A 599	-7.009	4.682	-12.355	1.00	0.00
ATOM	1273	N	TRP A 600	-5.374	0.197	-10.930	1.00	0.00

42/208

ATOM	1274	CA	TRP A 600	-5.750	-0.339	-9.618	1.00	0.00
ATOM	1275	C	TRP A 600	-5.235	0.537	-8.454	1.00	0.00
ATOM	1276	O	TRP A 600	-5.982	0.998	-7.602	1.00	0.00
ATOM	1277	CB	TRP A 600	-5.158	-1.745	-9.508	1.00	0.00
ATOM	1278	CG	TRP A 600	-5.055	-2.226	-8.069	1.00	0.00
ATOM	1279	CD1	TRP A 600	-3.885	-2.666	-7.450	1.00	0.00
ATOM	1280	CD2	TRP A 600	-6.086	-2.286	-7.065	1.00	0.00
ATOM	1281	NE1	TRP A 600	-4.138	-2.989	-6.162	1.00	0.00
ATOM	1282	CE2	TRP A 600	-5.478	-2.771	-5.881	1.00	0.00
ATOM	1283	CE3	TRP A 600	-7.415	-1.962	-7.073	1.00	0.00
ATOM	1284	CZ2	TRP A 600	-6.220	-2.924	-4.744	1.00	0.00
ATOM	1285	CZ3	TRP A 600	-8.169	-2.109	-5.914	1.00	0.00
ATOM	1286	CH2	TRP A 600	-7.572	-2.594	-4.754	1.00	0.00
ATOM	1287	HN	TRP A 600	-5.041	-0.407	-11.658	1.00	0.00
ATOM	1288	HA	TRP A 600	-6.840	-0.362	-9.586	1.00	0.00
ATOM	1289	IHB	TRP A 600	-4.152	-1.676	-9.917	1.00	0.00
ATOM	1290	2HB	TRP A 600	-5.714	-2.461	-10.115	1.00	0.00
ATOM	1291	HE3	TRP A 600	-7.881	-1.589	-7.972	1.00	0.00
ATOM	1292	HD1	TRP A 600	-2.918	-2.729	-7.926	1.00	0.00
ATOM	1293	HE1	TRP A 600	-3.470	-3.318	-5.525	1.00	0.00
ATOM	1294	HZ2	TRP A 600	-5.762	-3.299	-3.842	1.00	0.00
ATOM	1295	HZ3	TRP A 600	-9.212	-1.838	-5.907	1.00	0.00
ATOM	1296	HH2	TRP A 600	-8.161	-2.715	-3.864	1.00	0.00
ATOM	1297	N	MET A 601	-3.903	0.714	-8.453	1.00	0.00
ATOM	1298	CA	MET A 601	-3.290	1.376	-7.306	1.00	0.00
ATOM	1299	C	MET A 601	-3.711	2.849	-7.232	1.00	0.00
ATOM	1300	O	MET A 601	-3.783	3.435	-6.160	1.00	0.00
ATOM	1301	CB	MET A 601	-1.761	1.224	-7.356	1.00	0.00
ATOM	1302	CG	MET A 601	-1.317	-0.233	-7.166	1.00	0.00
ATOM	1303	SD	MET A 601	-1.813	-0.871	-5.552	1.00	0.00
ATOM	1304	CE	MET A 601	-0.700	-2.284	-5.450	1.00	0.00
ATOM	1305	HN	MET A 601	-3.367	0.312	-9.194	1.00	0.00
ATOM	1306	HA	MET A 601	-3.678	0.887	-6.410	1.00	0.00
ATOM	1307	IHB	MET A 601	-1.305	1.830	-6.572	1.00	0.00
ATOM	1308	2HB	MET A 601	-1.377	1.612	-8.300	1.00	0.00
ATOM	1309	IHG	MET A 601	-0.235	-0.297	-7.234	1.00	0.00
ATOM	1310	2HG	MET A 601	-1.700	-0.874	-7.957	1.00	0.00
ATOM	1311	IHE	MET A 601	-1.012	-3.065	-6.143	1.00	0.00
ATOM	1312	2HE	MET A 601	-0.682	-2.677	-4.433	1.00	0.00
ATOM	1313	3HE	MET A 601	0.315	-1.986	-5.713	1.00	0.00
ATOM	1314	N	PHE A 602	-4.012	3.399	-8.430	1.00	0.00
ATOM	1315	CA	PHE A 602	-4.329	4.792	-8.552	1.00	0.00
ATOM	1316	C	PHE A 602	-5.642	4.922	-7.841	1.00	0.00
ATOM	1317	O	PHE A 602	-5.808	5.741	-6.936	1.00	0.00
ATOM	1318	CB	PHE A 602	-4.600	5.152	-10.026	1.00	0.00
ATOM	1319	CG	PHE A 602	-4.341	6.595	-10.299	1.00	0.00
ATOM	1320	CD1	PHE A 602	-3.197	6.950	-10.976	1.00	0.00
ATOM	1321	CD2	PHE A 602	-5.191	7.584	-9.864	1.00	0.00
ATOM	1322	CE1	PHE A 602	-2.935	8.262	-11.292	1.00	0.00

43/208

ATOM	1323	CE2 PHE A 602	-4.909	8.902	-10.141	1.00	0.00
ATOM	1324	CZ PHE A 602	-3.804	9.242	-10.885	1.00	0.00
ATOM	1325	HN PHE A 602	-3.876	2.850	-9.254	1.00	0.00
ATOM	1326	HA PHE A 602	-3.478	5.353	-8.169	1.00	0.00
ATOM	1327	1HB PHE A 602	-5.640	4.934	-10.269	1.00	0.00
ATOM	1328	2HB PHE A 602	-3.955	4.556	-10.671	1.00	0.00
ATOM	1329	HD1 PHE A 602	-2.492	6.184	-11.265	1.00	0.00
ATOM	1330	HD2 PHE A 602	-6.079	7.328	-9.306	1.00	0.00
ATOM	1331	HE1 PHE A 602	-2.051	8.519	-11.857	1.00	0.00
ATOM	1332	HE2 PHE A 602	-5.562	9.677	-9.769	1.00	0.00
ATOM	1333	HZ PHE A 602	-3.622	10.274	-11.148	1.00	0.00
ATOM	1334	N LEU A 603	-6.582	4.031	-8.209	1.00	0.00
ATOM	1335	CA LEU A 603	-7.919	3.980	-7.692	1.00	0.00
ATOM	1336	C LEU A 603	-7.888	3.784	-6.209	1.00	0.00
ATOM	1337	O LEU A 603	-8.534	4.518	-5.462	1.00	0.00
ATOM	1338	CB LEU A 603	-8.662	2.763	-8.271	1.00	0.00
ATOM	1339	CG LEU A 603	-10.109	2.593	-7.789	1.00	0.00
ATOM	1340	CD1 LEU A 603	-11.000	3.712	-8.331	1.00	0.00
ATOM	1341	CD2 LEU A 603	-10.648	1.191	-8.117	1.00	0.00
ATOM	1342	HN LEU A 603	-6.327	3.352	-8.896	1.00	0.00
ATOM	1343	HA LEU A 603	-8.414	4.907	-7.979	1.00	0.00
ATOM	1344	1HB LEU A 603	-8.106	1.865	-8.005	1.00	0.00
ATOM	1345	2HB LEU A 603	-8.671	2.852	-9.356	1.00	0.00
ATOM	1346	HG LEU A 603	-10.132	2.607	-6.700	1.00	0.00
ATOM	1347	1HD1 LEU A 603	-10.542	4.183	-9.200	1.00	0.00
ATOM	1348	2HD1 LEU A 603	-11.146	4.478	-7.570	1.00	0.00
ATOM	1349	3HD1 LEU A 603	-11.966	3.310	-8.635	1.00	0.00
ATOM	1350	1HD2 LEU A 603	-10.043	0.423	-7.635	1.00	0.00
ATOM	1351	2HD2 LEU A 603	-10.618	1.018	-9.193	1.00	0.00
ATOM	1352	3HD2 LEU A 603	-11.672	1.088	-7.759	1.00	0.00
ATOM	1353	N MET A 604	-7.108	2.801	-5.735	1.00	0.00
ATOM	1354	CA MET A 604	-7.162	2.563	-4.295	1.00	0.00
ATOM	1355	C MET A 604	-6.553	3.736	-3.494	1.00	0.00
ATOM	1356	O MET A 604	-6.989	4.068	-2.394	1.00	0.00
ATOM	1357	CB MET A 604	-6.551	1.197	-3.954	1.00	0.00
ATOM	1358	CG MET A 604	-7.377	0.461	-2.891	1.00	0.00
ATOM	1359	SD MET A 604	-9.047	0.097	-3.483	1.00	0.00
ATOM	1360	CE MET A 604	-10.010	1.373	-2.647	1.00	0.00
ATOM	1361	HN MET A 604	-6.591	2.225	-6.370	1.00	0.00
ATOM	1362	HA MET A 604	-8.222	2.547	-4.050	1.00	0.00
ATOM	1363	1HB MET A 604	-5.513	1.302	-3.633	1.00	0.00
ATOM	1364	2HB MET A 604	-6.522	0.572	-4.849	1.00	0.00
ATOM	1365	1HG MET A 604	-7.413	1.016	-1.954	1.00	0.00
ATOM	1366	2HG MET A 604	-6.900	-0.491	-2.669	1.00	0.00
ATOM	1367	1HE MET A 604	-10.288	2.160	-3.348	1.00	0.00
ATOM	1368	2HE MET A 604	-9.473	1.797	-1.800	1.00	0.00
ATOM	1369	3HE MET A 604	-10.936	0.941	-2.272	1.00	0.00
ATOM	1370	N ALA A 605	-5.545	4.363	-4.137	1.00	0.00
ATOM	1371	CA ALA A 605	-4.874	5.506	-3.532	1.00	0.00

44/208

ATOM	1372	C	ALA A 605	-5.827	6.702	-3.362	1.00	0.00
ATOM	1373	O	ALA A 605	-5.878	7.310	-2.299	1.00	0.00
ATOM	1374	CB	ALA A 605	-3.646	5.903	-4.361	1.00	0.00
ATOM	1375	HN	ALA A 605	-5.229	4.030	-5.030	1.00	0.00
ATOM	1376	HA	ALA A 605	-4.552	5.187	-2.539	1.00	0.00
ATOM	1377	1HB	ALA A 605	-3.118	6.743	-3.908	1.00	0.00
ATOM	1378	2HB	ALA A 605	-3.918	6.189	-5.378	1.00	0.00
ATOM	1379	3HB	ALA A 605	-2.940	5.075	-4.429	1.00	0.00
ATOM	1380	N	PHE A 606	-6.591	7.014	-4.438	1.00	0.00
ATOM	1381	CA	PHE A 606	-7.447	8.165	-4.365	1.00	0.00
ATOM	1382	C	PHE A 606	-8.499	7.924	-3.332	1.00	0.00
ATOM	1383	O	PHE A 606	-8.914	8.843	-2.626	1.00	0.00
ATOM	1384	CB	PHE A 606	-8.128	8.482	-5.709	1.00	0.00
ATOM	1385	CG	PHE A 606	-8.764	9.826	-5.599	1.00	0.00
ATOM	1386	CD1	PHE A 606	-7.983	10.937	-5.380	1.00	0.00
ATOM	1387	CD2	PHE A 606	-10.075	10.011	-5.972	1.00	0.00
ATOM	1388	CE1	PHE A 606	-8.527	12.200	-5.390	1.00	0.00
ATOM	1389	CE2	PHE A 606	-10.612	11.275	-6.033	1.00	0.00
ATOM	1390	CZ	PHE A 606	-9.853	12.370	-5.702	1.00	0.00
ATOM	1391	HN	PHE A 606	-6.547	6.469	-5.275	1.00	0.00
ATOM	1392	HA	PHE A 606	-6.822	9.002	-4.055	1.00	0.00
ATOM	1393	1HB	PHE A 606	-8.890	7.736	-5.934	1.00	0.00
ATOM	1394	2HB	PHE A 606	-7.395	8.490	-6.515	1.00	0.00
ATOM	1395	HD1	PHE A 606	-6.926	10.816	-5.196	1.00	0.00
ATOM	1396	HD2	PHE A 606	-10.687	9.156	-6.219	1.00	0.00
ATOM	1397	HE1	PHE A 606	-7.912	13.056	-5.154	1.00	0.00
ATOM	1398	HE2	PHE A 606	-11.638	11.408	-6.342	1.00	0.00
ATOM	1399	HZ	PHE A 606	-10.295	13.356	-5.687	1.00	0.00
ATOM	1400	N	ALA A 607	-8.951	6.658	-3.251	1.00	0.00
ATOM	1401	CA	ALA A 607	-9.986	6.362	-2.267	1.00	0.00
ATOM	1402	C	ALA A 607	-9.485	6.561	-0.843	1.00	0.00
ATOM	1403	O	ALA A 607	-10.155	7.114	0.022	1.00	0.00
ATOM	1404	CB	ALA A 607	-10.490	4.929	-2.480	1.00	0.00
ATOM	1405	HN	ALA A 607	-8.636	5.964	-3.904	1.00	0.00
ATOM	1406	HA	ALA A 607	-10.759	7.108	-2.388	1.00	0.00
ATOM	1407	1HB	ALA A 607	-9.697	4.201	-2.307	1.00	0.00
ATOM	1408	2HB	ALA A 607	-10.839	4.790	-3.503	1.00	0.00
ATOM	1409	3HB	ALA A 607	-11.318	4.698	-1.809	1.00	0.00
ATOM	1410	N	LEU A 608	-8.251	6.069	-0.661	1.00	0.00
ATOM	1411	CA	LEU A 608	-7.589	6.185	0.626	1.00	0.00
ATOM	1412	C	LEU A 608	-7.499	7.666	1.051	1.00	0.00
ATOM	1413	O	LEU A 608	-7.854	8.037	2.161	1.00	0.00
ATOM	1414	CB	LEU A 608	-6.231	5.473	0.480	1.00	0.00
ATOM	1415	CG	LEU A 608	-5.341	5.404	1.730	1.00	0.00
ATOM	1416	CD1	LEU A 608	-4.488	6.666	1.889	1.00	0.00
ATOM	1417	CD2	LEU A 608	-6.131	5.062	3.000	1.00	0.00
ATOM	1418	HN	LEU A 608	-7.785	5.630	-1.434	1.00	0.00
ATOM	1419	HA	LEU A 608	-8.219	5.663	1.348	1.00	0.00
ATOM	1420	1HB	LEU A 608	-5.662	5.906	-0.342	1.00	0.00

45/208

ATOM	1421	2HB	LEU	A 608	-6.446	4.453	0.166	1.00	0.00
ATOM	1422	HG	LEU	A 608	-4.638	4.586	1.562	1.00	0.00
ATOM	1423	1HD1	LEU	A 608	-3.936	6.889	0.977	1.00	0.00
ATOM	1424	2HD1	LEU	A 608	-3.758	6.534	2.684	1.00	0.00
ATOM	1425	3HD1	LEU	A 608	-5.087	7.542	2.119	1.00	0.00
ATOM	1426	1HD2	LEU	A 608	-5.464	4.811	3.825	1.00	0.00
ATOM	1427	2HD2	LEU	A 608	-6.776	4.201	2.829	1.00	0.00
ATOM	1428	3HD2	LEU	A 608	-6.760	5.891	3.325	1.00	0.00
ATOM	1429	N	GLY	A 609	-7.042	8.497	0.093	1.00	0.00
ATOM	1430	CA	GLY	A 609	-6.823	9.887	0.364	1.00	0.00
ATOM	1431	C	GLY	A 609	-8.130	10.530	0.702	1.00	0.00
ATOM	1432	O	GLY	A 609	-8.225	11.332	1.631	1.00	0.00
ATOM	1433	HN	GLY	A 609	-6.813	8.122	-0.806	1.00	0.00
ATOM	1434	1HA	GLY	A 609	-6.401	10.344	-0.530	1.00	0.00
ATOM	1435	2HA	GLY	A 609	-6.138	9.963	1.208	1.00	0.00
ATOM	1436	N	TRP	A 610	-9.180	10.177	-0.058	1.00	0.00
ATOM	1437	CA	TRP	A 610	-10.495	10.719	0.121	1.00	0.00
ATOM	1438	C	TRP	A 610	-11.037	10.406	1.478	1.00	0.00
ATOM	1439	O	TRP	A 610	-11.582	11.277	2.154	1.00	0.00
ATOM	1440	CB	TRP	A 610	-11.473	10.139	-0.913	1.00	0.00
ATOM	1441	CG	TRP	A 610	-12.929	10.398	-0.623	1.00	0.00
ATOM	1442	CD1	TRP	A 610	-13.862	9.539	-0.122	1.00	0.00
ATOM	1443	CD2	TRP	A 610	-13.576	11.671	-0.753	1.00	0.00
ATOM	1444	NE1	TRP	A 610	-15.063	10.187	0.033	1.00	0.00
ATOM	1445	CE2	TRP	A 610	-14.899	11.503	-0.345	1.00	0.00
ATOM	1446	CE3	TRP	A 610	-13.106	12.882	-1.173	1.00	0.00
ATOM	1447	CZ2	TRP	A 610	-15.777	12.548	-0.356	1.00	0.00
ATOM	1448	CZ3	TRP	A 610	-13.993	13.934	-1.180	1.00	0.00
ATOM	1449	CH2	TRP	A 610	-15.303	13.769	-0.781	1.00	0.00
ATOM	1450	HN	TRP	A 610	-9.037	9.503	-0.783	1.00	0.00
ATOM	1451	HA	TRP	A 610	-10.415	11.800	0.008	1.00	0.00
ATOM	1452	1HB	TRP	A 610	-11.331	9.060	-0.961	1.00	0.00
ATOM	1453	2HB	TRP	A 610	-11.246	10.569	-1.887	1.00	0.00
ATOM	1454	HE3	TRP	A 610	-12.080	13.008	-1.487	1.00	0.00
ATOM	1455	HD1	TRP	A 610	-13.682	8.502	0.119	1.00	0.00
ATOM	1456	HE1	TRP	A 610	-15.894	9.783	0.357	1.00	0.00
ATOM	1457	HZ2	TRP	A 610	-16.803	12.422	-0.044	1.00	0.00
ATOM	1458	HZ3	TRP	A 610	-13.657	14.907	-1.504	1.00	0.00
ATOM	1459	HH2	TRP	A 610	-15.971	14.617	-0.802	1.00	0.00
ATOM	1460	N	ARG	A 611	-10.908	9.137	1.904	1.00	0.00
ATOM	1461	CA	ARG	A 611	-11.485	8.823	3.212	1.00	0.00
ATOM	1462	C	ARG	A 611	-10.630	9.382	4.363	1.00	0.00
ATOM	1463	O	ARG	A 611	-11.108	9.620	5.463	1.00	0.00
ATOM	1464	CB	ARG	A 611	-11.704	7.323	3.367	1.00	0.00
ATOM	1465	CG	ARG	A 611	-12.850	6.806	2.484	1.00	0.00
ATOM	1466	CD	ARG	A 611	-13.346	5.416	2.901	1.00	0.00
ATOM	1467	NE	ARG	A 611	-12.276	4.442	2.750	1.00	0.00
ATOM	1468	CZ	ARG	A 611	-11.360	4.161	3.704	1.00	0.00
ATOM	1469	NH1	ARG	A 611	-11.429	4.663	4.939	1.00	0.00

46/208

ATOM	1470	NH2	ARG A 611	-10.349	3.373	3.370	1.00	0.00
ATOM	1471	HN	ARG A 611	-10.461	8.449	1.327	1.00	0.00
ATOM	1472	HA	ARG A 611	-12.458	9.315	3.274	1.00	0.00
ATOM	1473	IHB	ARG A 611	-11.960	7.134	4.408	1.00	0.00
ATOM	1474	2HB	ARG A 611	-10.775	6.791	3.162	1.00	0.00
ATOM	1475	IHG	ARG A 611	-12.533	6.795	1.440	1.00	0.00
ATOM	1476	2HG	ARG A 611	-13.693	7.495	2.541	1.00	0.00
ATOM	1477	IHD	ARG A 611	-14.154	5.084	2.248	1.00	0.00
ATOM	1478	2HD	ARG A 611	-13.724	5.389	3.923	1.00	0.00
ATOM	1479	HE	ARG A 611	-12.203	4.016	1.848	1.00	0.00
ATOM	1480	IHH1	ARG A 611	-12.239	5.161	5.293	1.00	0.00
ATOM	1481	2HH1	ARG A 611	-10.631	4.578	5.546	1.00	0.00
ATOM	1482	IHH2	ARG A 611	-9.738	2.982	4.066	1.00	0.00
ATOM	1483	2HH2	ARG A 611	-10.158	3.134	2.412	1.00	0.00
ATOM	1484	N	SER A 612	-9.356	9.624	4.043	1.00	0.00
ATOM	1485	CA	SER A 612	-8.434	10.203	4.984	1.00	0.00
ATOM	1486	C	SER A 612	-8.651	11.664	5.221	1.00	0.00
ATOM	1487	O	SER A 612	-8.081	12.237	6.147	1.00	0.00
ATOM	1488	CB	SER A 612	-6.965	10.024	4.572	1.00	0.00
ATOM	1489	OG	SER A 612	-6.605	8.656	4.662	1.00	0.00
ATOM	1490	HN	SER A 612	-9.005	9.410	3.133	1.00	0.00
ATOM	1491	HA	SER A 612	-8.617	9.712	5.940	1.00	0.00
ATOM	1492	IHB	SER A 612	-6.313	10.595	5.233	1.00	0.00
ATOM	1493	2HB	SER A 612	-6.817	10.351	3.543	1.00	0.00
ATOM	1494	HG	SER A 612	-5.753	8.571	4.254	1.00	0.00
ATOM	1495	N	TYR A 613	-9.470	12.302	4.372	1.00	0.00
ATOM	1496	CA	TYR A 613	-9.629	13.727	4.326	1.00	0.00
ATOM	1497	C	TYR A 613	-9.847	14.349	5.675	1.00	0.00
ATOM	1498	O	TYR A 613	-9.040	15.171	6.102	1.00	0.00
ATOM	1499	CB	TYR A 613	-10.852	14.052	3.449	1.00	0.00
ATOM	1500	CG	TYR A 613	-10.984	15.506	3.166	1.00	0.00
ATOM	1501	CD1	TYR A 613	-11.417	16.382	4.134	1.00	0.00
ATOM	1502	CD2	TYR A 613	-10.952	15.928	1.857	1.00	0.00
ATOM	1503	CE1	TYR A 613	-11.756	17.674	3.804	1.00	0.00
ATOM	1504	CE2	TYR A 613	-11.302	17.211	1.518	1.00	0.00
ATOM	1505	CZ	TYR A 613	-11.707	18.087	2.494	1.00	0.00
ATOM	1506	OH	TYR A 613	-12.108	19.393	2.145	1.00	0.00
ATOM	1507	HN	TYR A 613	-10.002	11.750	3.732	1.00	0.00
ATOM	1508	HA	TYR A 613	-8.718	14.150	3.903	1.00	0.00
ATOM	1509	IHB	TYR A 613	-11.757	13.718	3.955	1.00	0.00
ATOM	1510	2HB	TYR A 613	-10.763	13.525	2.499	1.00	0.00
ATOM	1511	HD1	TYR A 613	-11.492	16.053	5.160	1.00	0.00
ATOM	1512	HE1	TYR A 613	-12.060	18.366	4.576	1.00	0.00
ATOM	1513	HD2	TYR A 613	-10.647	15.238	1.084	1.00	0.00
ATOM	1514	HE2	TYR A 613	-11.260	17.530	0.487	1.00	0.00
ATOM	1515	HH	TYR A 613	-11.566	20.023	2.601	1.00	0.00
ATOM	1516	N	ARG A 614	-10.901	13.979	6.422	1.00	0.00
ATOM	1517	CA	ARG A 614	-11.083	14.637	7.689	1.00	0.00
ATOM	1518	C	ARG A 614	-10.061	14.304	8.732	1.00	0.00

SUBSTITUTE SHEET (RULE 26)



47/208

ATOM	1519	O	ARG A 614	-9.739	15.139	9.577	1.00	0.00
ATOM	1520	CB	ARG A 614	-12.507	14.538	8.277	1.00	0.00
ATOM	1521	CG	ARG A 614	-13.137	13.148	8.278	1.00	0.00
ATOM	1522	CD	ARG A 614	-12.266	12.021	8.819	1.00	0.00
ATOM	1523	NE	ARG A 614	-13.095	10.787	8.732	1.00	0.00
ATOM	1524	CZ	ARG A 614	-13.441	10.285	7.509	1.00	0.00
ATOM	1525	NH1	ARG A 614	-13.181	11.003	6.378	1.00	0.00
ATOM	1526	NH2	ARG A 614	-14.083	9.085	7.418	1.00	0.00
ATOM	1527	HN	ARG A 614	-11.535	13.273	6.108	1.00	0.00
ATOM	1528	HA	ARG A 614	-10.827	15.683	7.525	1.00	0.00
ATOM	1529	1HB	ARG A 614	-13.154	15.201	7.705	1.00	0.00
ATOM	1530	2HB	ARG A 614	-12.472	14.894	9.305	1.00	0.00
ATOM	1531	1HG	ARG A 614	-13.411	12.900	7.255	1.00	0.00
ATOM	1532	2HG	ARG A 614	-14.045	13.190	8.878	1.00	0.00
ATOM	1533	1HD	ARG A 614	-11.998	12.183	9.862	1.00	0.00
ATOM	1534	2HD	ARG A 614	-11.371	11.878	8.215	1.00	0.00
ATOM	1535	HE	ARG A 614	-13.400	10.327	9.566	1.00	0.00
ATOM	1536	1HH1	ARG A 614	-12.608	11.822	6.425	1.00	0.00
ATOM	1537	2HH1	ARG A 614	-13.563	10.711	5.501	1.00	0.00
ATOM	1538	1HH2	ARG A 614	-14.302	8.571	8.247	1.00	0.00
ATOM	1539	2HH2	ARG A 614	-14.335	8.719	6.522	1.00	0.00
ATOM	1540	N	GLN A 615	-9.518	13.078	8.712	1.00	0.00
ATOM	1541	CA	GLN A 615	-8.577	12.675	9.719	1.00	0.00
ATOM	1542	C	GLN A 615	-7.221	13.187	9.341	1.00	0.00
ATOM	1543	O	GLN A 615	-6.452	12.503	8.664	1.00	0.00
ATOM	1544	CB	GLN A 615	-8.505	11.148	9.800	1.00	0.00
ATOM	1545	CG	GLN A 615	-9.842	10.488	10.155	1.00	0.00
ATOM	1546	CD	GLN A 615	-10.217	10.878	11.579	1.00	0.00
ATOM	1547	OE1	GLN A 615	-9.475	11.575	12.269	1.00	0.00
ATOM	1548	NE2	GLN A 615	-11.411	10.413	12.035	1.00	0.00
ATOM	1549	HN	GLN A 615	-9.771	12.437	7.987	1.00	0.00
ATOM	1550	HA	GLN A 615	-8.916	13.095	10.666	1.00	0.00
ATOM	1551	1HB	GLN A 615	-7.768	10.872	10.553	1.00	0.00
ATOM	1552	2HB	GLN A 615	-8.171	10.763	8.837	1.00	0.00
ATOM	1553	1HG	GLN A 615	-9.759	9.403	10.093	1.00	0.00
ATOM	1554	2HG	GLN A 615	-10.624	10.826	9.475	1.00	0.00
ATOM	1555	1HE2	GLN A 615	-11.913	9.731	11.502	1.00	0.00
ATOM	1556	2HE2	GLN A 615	-11.800	10.740	12.895	1.00	0.00
ATOM	1557	N	SER A 616	-6.865	14.393	9.825	1.00	0.00
ATOM	1558	CA	SER A 616	-5.661	15.027	9.371	1.00	0.00
ATOM	1559	C	SER A 616	-4.431	14.879	10.213	1.00	0.00
ATOM	1560	O	SER A 616	-4.477	14.649	11.421	1.00	0.00
ATOM	1561	CB	SER A 616	-5.840	16.541	9.163	1.00	0.00
ATOM	1562	OG	SER A 616	-4.622	17.122	8.721	1.00	0.00
ATOM	1563	HN	SER A 616	-7.443	14.848	10.504	1.00	0.00
ATOM	1564	HA	SER A 616	-5.388	14.547	8.432	1.00	0.00
ATOM	1565	1HB	SER A 616	-6.127	17.020	10.099	1.00	0.00
ATOM	1566	2HB	SER A 616	-6.603	16.731	8.407	1.00	0.00
ATOM	1567	HG	SER A 616	-4.480	16.816	7.835	1.00	0.00

48/208

ATOM	1568	N	SER A 617	-3.286	14.953	9.504	1.00	0.00
ATOM	1569	CA	SER A 617	-1.945	15.132	9.987	1.00	0.00
ATOM	1570	C	SER A 617	-1.302	14.020	10.728	1.00	0.00
ATOM	1571	O	SER A 617	-0.091	13.825	10.625	1.00	0.00
ATOM	1572	CB	SER A 617	-1.804	16.386	10.867	1.00	0.00
ATOM	1573	OG	SER A 617	-2.536	16.222	12.072	1.00	0.00
ATOM	1574	HN	SER A 617	-3.383	14.873	8.515	1.00	0.00
ATOM	1575	HA	SER A 617	-1.303	15.212	9.110	1.00	0.00
ATOM	1576	IHB	SER A 617	-2.195	17.260	10.346	1.00	0.00
ATOM	1577	2HB	SER A 617	-0.757	16.553	11.123	1.00	0.00
ATOM	1578	HG	SER A 617	-2.282	15.383	12.433	1.00	0.00
ATOM	1579	N	ALA A 618	-2.055	13.181	11.440	1.00	0.00
ATOM	1580	CA	ALA A 618	-1.297	12.170	12.109	1.00	0.00
ATOM	1581	C	ALA A 618	-1.203	11.075	11.117	1.00	0.00
ATOM	1582	O	ALA A 618	-1.451	9.937	11.510	1.00	0.00
ATOM	1583	CB	ALA A 618	-2.014	11.587	13.336	1.00	0.00
ATOM	1584	HN	ALA A 618	-3.048	13.253	11.500	1.00	0.00
ATOM	1585	HA	ALA A 618	-0.359	12.634	12.411	1.00	0.00
ATOM	1586	IHB	ALA A 618	-2.962	11.133	13.049	1.00	0.00
ATOM	1587	2HB	ALA A 618	-2.222	12.375	14.060	1.00	0.00
ATOM	1588	3HB	ALA A 618	-1.398	10.816	13.800	1.00	0.00
ATOM	1589	N	ASN A 619	-0.796	11.421	9.859	1.00	0.00
ATOM	1590	CA	ASN A 619	-0.825	10.611	8.670	1.00	0.00
ATOM	1591	C	ASN A 619	-2.027	9.830	8.892	1.00	0.00
ATOM	1592	O	ASN A 619	-1.981	8.604	8.928	1.00	0.00
ATOM	1593	CB	ASN A 619	0.358	9.664	8.464	1.00	0.00
ATOM	1594	CG	ASN A 619	0.176	8.729	7.272	1.00	0.00
ATOM	1595	OD1	ASN A 619	0.496	7.545	7.372	1.00	0.00
ATOM	1596	ND2	ASN A 619	-0.308	9.261	6.121	1.00	0.00
ATOM	1597	HN	ASN A 619	-0.437	12.346	9.753	1.00	0.00
ATOM	1598	HA	ASN A 619	-0.872	11.312	7.837	1.00	0.00
ATOM	1599	IHB	ASN A 619	0.487	9.051	9.355	1.00	0.00
ATOM	1600	2HB	ASN A 619	1.262	10.248	8.298	1.00	0.00
ATOM	1601	IHD2	ASN A 619	-0.165	8.782	5.255	1.00	0.00
ATOM	1602	2HD2	ASN A 619	-0.808	10.126	6.121	1.00	0.00
ATOM	1603	N	LEU A 620	-3.132	10.545	9.137	1.00	0.00
ATOM	1604	CA	LEU A 620	-4.225	9.747	9.520	1.00	0.00
ATOM	1605	C	LEU A 620	-4.730	9.261	8.225	1.00	0.00
ATOM	1606	O	LEU A 620	-5.412	9.965	7.478	1.00	0.00
ATOM	1607	CB	LEU A 620	-5.288	10.498	10.341	1.00	0.00
ATOM	1608	CG	LEU A 620	-6.190	9.548	11.155	1.00	0.00
ATOM	1609	CD1	LEU A 620	-7.024	10.322	12.191	1.00	0.00
ATOM	1610	CD2	LEU A 620	-7.029	8.637	10.242	1.00	0.00
ATOM	1611	HN	LEU A 620	-3.174	11.538	9.056	1.00	0.00
ATOM	1612	HA	LEU A 620	-3.815	8.927	10.108	1.00	0.00
ATOM	1613	IHB	LEU A 620	-5.910	11.082	9.664	1.00	0.00
ATOM	1614	2HB	LEU A 620	-4.789	11.183	11.024	1.00	0.00
ATOM	1615	HG	LEU A 620	-5.570	8.814	11.667	1.00	0.00
ATOM	1616	IHD1	LEU A 620	-6.943	11.397	12.025	1.00	0.00

49/208

ATOM 1617 2HD1 LEU A 620	-6.666	10.109	13.198	1.00	0.00
ATOM 1618 3HD1 LEU A 620	-8.075	10.047	12.110	1.00	0.00
ATOM 1619 1HD2 LEU A 620	-6.433	7.798	9.883	1.00	0.00
ATOM 1620 2HD2 LEU A 620	-7.383	9.195	9.376	1.00	0.00
ATOM 1621 3HD2 LEU A 620	-7.880	8.235	10.792	1.00	0.00
ATOM 1622 N LEU A 621	-4.250	8.020	7.935	1.00	0.00
ATOM 1623 CA LEU A 621	-4.711	7.307	6.773	1.00	0.00
ATOM 1624 C LEU A 621	-5.670	6.299	7.278	1.00	0.00
ATOM 1625 O LEU A 621	-5.333	5.304	7.915	1.00	0.00
ATOM 1626 CB LEU A 621	-3.721	6.649	5.792	1.00	0.00
ATOM 1627 CG LEU A 621	-2.520	7.497	5.409	1.00	0.00
ATOM 1628 CD1 LEU A 621	-1.471	6.654	4.663	1.00	0.00
ATOM 1629 CD2 LEU A 621	-2.900	8.754	4.603	1.00	0.00
ATOM 1630 HN LEU A 621	-3.596	7.614	8.584	1.00	0.00
ATOM 1631 HA LEU A 621	-5.268	8.045	6.264	1.00	0.00
ATOM 1632 1HB LEU A 621	-4.261	6.377	4.887	1.00	0.00
ATOM 1633 2HB LEU A 621	-3.363	5.699	6.173	1.00	0.00
ATOM 1634 HG LEU A 621	-2.110	7.785	6.370	1.00	0.00
ATOM 1635 1HD1 LEU A 621	-1.902	6.153	3.797	1.00	0.00
ATOM 1636 2HD1 LEU A 621	-1.059	5.885	5.317	1.00	0.00
ATOM 1637 3HD1 LEU A 621	-0.638	7.255	4.304	1.00	0.00
ATOM 1638 1HD2 LEU A 621	-3.553	9.411	5.177	1.00	0.00
ATOM 1639 2HD2 LEU A 621	-3.386	8.494	3.666	1.00	0.00
ATOM 1640 3HD2 LEU A 621	-2.029	9.340	4.318	1.00	0.00
ATOM 1641 N CYS A 622	-6.921	6.628	6.985	1.00	0.00
ATOM 1642 CA CYS A 622	-7.895	5.726	7.488	1.00	0.00
ATOM 1643 C CYS A 622	-7.990	4.641	6.469	1.00	0.00
ATOM 1644 O CYS A 622	-8.809	4.706	5.555	1.00	0.00
ATOM 1645 CB CYS A 622	-9.280	6.384	7.620	1.00	0.00
ATOM 1646 SG CYS A 622	-10.556	5.264	8.264	1.00	0.00
ATOM 1647 HN CYS A 622	-7.194	7.414	6.431	1.00	0.00
ATOM 1648 HA CYS A 622	-7.541	5.391	8.463	1.00	0.00
ATOM 1649 1HB CYS A 622	-9.601	6.735	6.640	1.00	0.00
ATOM 1650 2HB CYS A 622	-9.206	7.236	8.294	1.00	0.00
ATOM 1651 HG CYS A 622	-10.037	4.510	9.236	1.00	0.00
ATOM 1652 N PHE A 623	-7.120	3.616	6.603	1.00	0.00
ATOM 1653 CA PHE A 623	-7.232	2.532	5.627	1.00	0.00
ATOM 1654 C PHE A 623	-8.592	1.854	5.778	1.00	0.00
ATOM 1655 O PHE A 623	-9.217	1.491	4.790	1.00	0.00
ATOM 1656 CB PHE A 623	-6.106	1.494	5.696	1.00	0.00
ATOM 1657 CG PHE A 623	-4.839	1.984	5.052	1.00	0.00
ATOM 1658 CD1 PHE A 623	-3.876	2.685	5.771	1.00	0.00
ATOM 1659 CD2 PHE A 623	-4.619	1.727	3.704	1.00	0.00
ATOM 1660 CE1 PHE A 623	-2.708	3.107	5.147	1.00	0.00
ATOM 1661 CE2 PHE A 623	-3.457	2.152	3.080	1.00	0.00
ATOM 1662 CZ PHE A 623	-2.497	2.843	3.801	1.00	0.00
ATOM 1663 HN PHE A 623	-6.464	3.646	7.361	1.00	0.00
ATOM 1664 HA PHE A 623	-7.218	2.992	4.638	1.00	0.00
ATOM 1665 1HB PHE A 623	-6.416	0.606	5.143	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

50/208

ATOM	1666	2HB	PHE A 623	-5.923	1.144	6.704	1.00	0.00
ATOM	1667	HD1	PHE A 623	-4.032	2.911	6.817	1.00	0.00
ATOM	1668	HD2	PHE A 623	-5.362	1.190	3.135	1.00	0.00
ATOM	1669	HE1	PHE A 623	-1.954	3.639	5.703	1.00	0.00
ATOM	1670	HE2	PHE A 623	-3.306	1.942	2.035	1.00	0.00
ATOM	1671	HZ	PHE A 623	-1.590	3.174	3.318	1.00	0.00
ATOM	1672	N	ALA A 624	-9.041	1.779	7.044	1.00	0.00
ATOM	1673	CA	ALA A 624	-10.350	1.267	7.317	1.00	0.00
ATOM	1674	C	ALA A 624	-10.855	2.038	8.493	1.00	0.00
ATOM	1675	O	ALA A 624	-10.065	2.613	9.241	1.00	0.00
ATOM	1676	CB	ALA A 624	-10.355	-0.217	7.721	1.00	0.00
ATOM	1677	HN	ALA A 624	-8.434	1.998	7.809	1.00	0.00
ATOM	1678	HA	ALA A 624	-10.933	1.407	6.407	1.00	0.00
ATOM	1679	IHB	ALA A 624	-10.609	-0.329	8.775	1.00	0.00
ATOM	1680	2HB	ALA A 624	-9.368	-0.653	7.564	1.00	0.00
ATOM	1681	3HB	ALA A 624	-11.094	-0.764	7.136	1.00	0.00
ATOM	1682	N	PRO A 625	-12.151	2.098	8.664	1.00	0.00
ATOM	1683	CA	PRO A 625	-12.727	2.784	9.789	1.00	0.00
ATOM	1684	C	PRO A 625	-12.116	2.154	10.996	1.00	0.00
ATOM	1685	O	PRO A 625	-11.963	2.805	12.029	1.00	0.00
ATOM	1686	CB	PRO A 625	-14.224	2.503	9.706	1.00	0.00
ATOM	1687	CG	PRO A 625	-14.283	1.125	9.020	1.00	0.00
ATOM	1688	CD	PRO A 625	-13.055	1.114	8.094	1.00	0.00
ATOM	1689	IHD	PRO A 625	-12.583	0.132	8.076	1.00	0.00
ATOM	1690	2HD	PRO A 625	-13.327	1.393	7.076	1.00	0.00
ATOM	1691	HA	PRO A 625	-12.524	3.853	9.724	1.00	0.00
ATOM	1692	IHB	PRO A 625	-14.739	3.261	9.117	1.00	0.00
ATOM	1693	2HB	PRO A 625	-14.679	2.473	10.696	1.00	0.00
ATOM	1694	IHG	PRO A 625	-14.230	0.320	9.753	1.00	0.00
ATOM	1695	2HG	PRO A 625	-15.205	1.009	8.452	1.00	0.00
ATOM	1696	N	ASP A 626	-11.833	0.854	10.863	1.00	0.00
ATOM	1697	CA	ASP A 626	-11.223	-0.014	11.814	1.00	0.00
ATOM	1698	C	ASP A 626	-9.743	0.240	11.957	1.00	0.00
ATOM	1699	O	ASP A 626	-9.180	0.039	13.029	1.00	0.00
ATOM	1700	CB	ASP A 626	-11.465	-1.471	11.380	1.00	0.00
ATOM	1701	CG	ASP A 626	-10.953	-2.418	12.437	1.00	0.00
ATOM	1702	OD1	ASP A 626	-9.716	-2.411	12.662	1.00	0.00
ATOM	1703	OD2	ASP A 626	-11.780	-3.159	13.032	1.00	0.00
ATOM	1704	HN	ASP A 626	-12.081	0.441	9.989	1.00	0.00
ATOM	1705	HA	ASP A 626	-11.677	0.186	12.785	1.00	0.00
ATOM	1706	IHB	ASP A 626	-10.944	-1.674	10.445	1.00	0.00
ATOM	1707	2HB	ASP A 626	-12.532	-1.647	11.239	1.00	0.00
ATOM	1708	N	LEU A 627	-9.066	0.665	10.865	1.00	0.00
ATOM	1709	CA	LEU A 627	-7.633	0.818	10.880	1.00	0.00
ATOM	1710	C	LEU A 627	-7.271	2.255	10.627	1.00	0.00
ATOM	1711	O	LEU A 627	-7.550	2.793	9.558	1.00	0.00
ATOM	1712	CB	LEU A 627	-7.009	-0.060	9.768	1.00	0.00
ATOM	1713	CG	LEU A 627	-5.475	-0.052	9.587	1.00	0.00
ATOM	1714	CD1	LEU A 627	-4.957	1.295	9.077	1.00	0.00

51/208

ATOM 1715 CD2 LEU A 627	-4.745	-0.561	10.841	1.00	0.00
ATOM 1716 HN LEU A 627	-9.573	0.878	10.029	1.00	0.00
ATOM 1717 HA LEU A 627	-7.280	0.508	11.864	1.00	0.00
ATOM 1718 1HB LEU A 627	-7.448	0.254	8.824	1.00	0.00
ATOM 1719 2HB LEU A 627	-7.306	-1.088	9.963	1.00	0.00
ATOM 1720 HG LEU A 627	-5.197	-0.831	8.878	1.00	0.00
ATOM 1721 1HD1 LEU A 627	-4.551	1.887	9.897	1.00	0.00
ATOM 1722 2HD1 LEU A 627	-5.768	1.862	8.621	1.00	0.00
ATOM 1723 3HD1 LEU A 627	-4.163	1.140	8.347	1.00	0.00
ATOM 1724 1HD2 LEU A 627	-5.167	-1.509	11.174	1.00	0.00
ATOM 1725 2HD2 LEU A 627	-4.846	0.158	11.653	1.00	0.00
ATOM 1726 3HD2 LEU A 627	-3.689	-0.721	10.622	1.00	0.00
ATOM 1727 N ILE A 628	-6.627	2.909	11.619	1.00	0.00
ATOM 1728 CA ILE A 628	-6.196	4.272	11.489	1.00	0.00
ATOM 1729 C ILE A 628	-4.708	4.248	11.691	1.00	0.00
ATOM 1730 O ILE A 628	-4.206	3.906	12.759	1.00	0.00
ATOM 1731 CB ILE A 628	-6.840	5.162	12.519	1.00	0.00
ATOM 1732 CG1 ILE A 628	-6.414	6.624	12.342	1.00	0.00
ATOM 1733 CG2 ILE A 628	-6.587	4.587	13.923	1.00	0.00
ATOM 1734 CD1 ILE A 628	-7.235	7.570	13.214	1.00	0.00
ATOM 1735 HN ILE A 628	-6.445	2.426	12.474	1.00	0.00
ATOM 1736 HA ILE A 628	-6.467	4.596	10.485	1.00	0.00
ATOM 1737 HB ILE A 628	-7.912	5.225	12.334	1.00	0.00
ATOM 1738 1HG2 ILE A 628	-5.586	4.844	14.270	1.00	0.00
ATOM 1739 2HG2 ILE A 628	-6.669	3.500	13.904	1.00	0.00
ATOM 1740 3HG2 ILE A 628	-7.305	4.997	14.633	1.00	0.00
ATOM 1741 1HG1 ILE A 628	-6.534	6.906	11.297	1.00	0.00
ATOM 1742 2HG1 ILE A 628	-5.361	6.722	12.604	1.00	0.00
ATOM 1743 1HD1 ILE A 628	-7.708	7.028	14.033	1.00	0.00
ATOM 1744 2HD1 ILE A 628	-8.022	8.039	12.622	1.00	0.00
ATOM 1745 3HD1 ILE A 628	-6.593	8.338	13.644	1.00	0.00
ATOM 1746 N ILE A 629	-3.950	4.627	10.651	1.00	0.00
ATOM 1747 CA ILE A 629	-2.526	4.519	10.716	1.00	0.00
ATOM 1748 C ILE A 629	-2.067	5.921	10.908	1.00	0.00
ATOM 1749 O ILE A 629	-2.791	6.847	10.547	1.00	0.00
ATOM 1750 CB ILE A 629	-2.017	3.951	9.416	1.00	0.00
ATOM 1751 CG1 ILE A 629	-0.621	3.322	9.516	1.00	0.00
ATOM 1752 CG2 ILE A 629	-2.118	5.071	8.367	1.00	0.00
ATOM 1753 CD1 ILE A 629	0.507	4.329	9.632	1.00	0.00
ATOM 1754 HN ILE A 629	-4.384	4.987	9.826	1.00	0.00
ATOM 1755 HA ILE A 629	-2.282	3.862	11.551	1.00	0.00
ATOM 1756 HB ILE A 629	-2.617	3.092	9.115	1.00	0.00
ATOM 1757 1HG2 ILE A 629	-1.666	5.990	8.740	1.00	0.00
ATOM 1758 2HG2 ILE A 629	-3.164	5.279	8.139	1.00	0.00
ATOM 1759 3HG2 ILE A 629	-1.594	4.783	7.456	1.00	0.00
ATOM 1760 1HG1 ILE A 629	-0.451	2.712	8.629	1.00	0.00
ATOM 1761 2HG1 ILE A 629	-0.596	2.671	10.389	1.00	0.00
ATOM 1762 1HD1 ILE A 629	0.483	4.823	10.604	1.00	0.00
ATOM 1763 2HD1 ILE A 629	0.409	5.095	8.862	1.00	0.00

52/208

ATOM	1764	3HD1 ILE A 629	1.470	3.829	9.532	1.00	0.00
ATOM	1765	N ASN A 630	-0.885	6.114	11.532	1.00	0.00
ATOM	1766	CA ASN A 630	-0.400	7.444	11.749	1.00	0.00
ATOM	1767	C ASN A 630	0.924	7.601	11.071	1.00	0.00
ATOM	1768	O ASN A 630	1.551	6.630	10.661	1.00	0.00
ATOM	1769	CB ASN A 630	-0.253	7.854	13.235	1.00	0.00
ATOM	1770	CG ASN A 630	0.838	7.047	13.930	1.00	0.00
ATOM	1771	OD1 ASN A 630	1.458	6.163	13.344	1.00	0.00
ATOM	1772	ND2 ASN A 630	1.082	7.357	15.231	1.00	0.00
ATOM	1773	HN ASN A 630	-0.349	5.328	11.841	1.00	0.00
ATOM	1774	HA ASN A 630	-1.110	8.108	11.256	1.00	0.00
ATOM	1775	1HB ASN A 630	-1.194	7.683	13.759	1.00	0.00
ATOM	1776	2HB ASN A 630	0.006	8.910	13.302	1.00	0.00
ATOM	1777	1HD2 ASN A 630	1.675	6.766	15.779	1.00	0.00
ATOM	1778	2HD2 ASN A 630	0.680	8.168	15.655	1.00	0.00
ATOM	1779	N GLU A 631	1.406	8.849	10.956	1.00	0.00
ATOM	1780	CA GLU A 631	2.599	9.081	10.196	1.00	0.00
ATOM	1781	C GLU A 631	3.753	8.273	10.685	1.00	0.00
ATOM	1782	O GLU A 631	4.423	7.610	9.898	1.00	0.00
ATOM	1783	CB GLU A 631	2.986	10.570	10.200	1.00	0.00
ATOM	1784	CG GLU A 631	4.040	10.927	9.155	1.00	0.00
ATOM	1785	CD GLU A 631	3.969	12.424	8.908	1.00	0.00
ATOM	1786	OE1 GLU A 631	4.594	12.887	7.918	1.00	0.00
ATOM	1787	OE2 GLU A 631	3.280	13.124	9.698	1.00	0.00
ATOM	1788	HN GLU A 631	0.934	9.612	11.398	1.00	0.00
ATOM	1789	HA GLU A 631	2.402	8.742	9.179	1.00	0.00
ATOM	1790	1HB GLU A 631	3.370	10.829	11.185	1.00	0.00
ATOM	1791	2HB GLU A 631	2.093	11.164	10.013	1.00	0.00
ATOM	1792	1HG GLU A 631	3.847	10.399	8.221	1.00	0.00
ATOM	1793	2HG GLU A 631	5.036	10.667	9.511	1.00	0.00
ATOM	1794	N GLN A 632	3.989	8.256	12.002	1.00	0.00
ATOM	1795	CA GLN A 632	5.122	7.551	12.527	1.00	0.00
ATOM	1796	C GLN A 632	5.005	6.083	12.267	1.00	0.00
ATOM	1797	O GLN A 632	6.003	5.400	12.040	1.00	0.00
ATOM	1798	CB GLN A 632	5.289	7.747	14.043	1.00	0.00
ATOM	1799	CG GLN A 632	5.656	9.183	14.423	1.00	0.00
ATOM	1800	CD GLN A 632	5.770	9.271	15.938	1.00	0.00
ATOM	1801	OE1 GLN A 632	5.297	10.231	16.543	1.00	0.00
ATOM	1802	NE2 GLN A 632	6.417	8.255	16.568	1.00	0.00
ATOM	1803	HN GLN A 632	3.371	8.738	12.623	1.00	0.00
ATOM	1804	HA GLN A 632	5.998	7.930	12.000	1.00	0.00
ATOM	1805	1HB GLN A 632	6.071	7.077	14.400	1.00	0.00
ATOM	1806	2HB GLN A 632	4.357	7.478	14.538	1.00	0.00
ATOM	1807	1HG GLN A 632	4.886	9.875	14.081	1.00	0.00
ATOM	1808	2HG GLN A 632	6.610	9.463	13.975	1.00	0.00
ATOM	1809	1HE2 GLN A 632	6.919	7.578	16.030	1.00	0.00
ATOM	1810	2HE2 GLN A 632	6.402	8.170	17.564	1.00	0.00
ATOM	1811	N ARG A 633	3.764	5.568	12.261	1.00	0.00
ATOM	1812	CA ARG A 633	3.523	4.160	12.139	1.00	0.00

53/208

ATOM 1813 C ARG A 633	4.131	3.680	10.869	1.00	0.00
ATOM 1814 O ARG A 633	4.547	2.529	10.774	1.00	0.00
ATOM 1815 CB ARG A 633	2.030	3.797	12.093	1.00	0.00
ATOM 1816 CG ARG A 633	1.725	2.310	12.292	1.00	0.00
ATOM 1817 CD ARG A 633	1.890	1.851	13.742	1.00	0.00
ATOM 1818 NE ARG A 633	1.264	2.893	14.605	1.00	0.00
ATOM 1819 CZ ARG A 633	-0.083	2.891	14.828	1.00	0.00
ATOM 1820 NH1 ARG A 633	-0.871	1.932	14.259	1.00	0.00
ATOM 1821 NH2 ARG A 633	-0.645	3.856	15.614	1.00	0.00
ATOM 1822 HN ARG A 633	2.984	6.188	12.345	1.00	0.00
ATOM 1823 HA ARG A 633	3.994	3.689	13.001	1.00	0.00
ATOM 1824 IHB ARG A 633	1.631	4.103	11.127	1.00	0.00
ATOM 1825 2HB ARG A 633	1.515	4.361	12.870	1.00	0.00
ATOM 1826 IHG ARG A 633	2.393	1.727	11.660	1.00	0.00
ATOM 1827 2HG ARG A 633	0.700	2.117	11.977	1.00	0.00
ATOM 1828 IHD ARG A 633	2.941	1.769	14.017	1.00	0.00
ATOM 1829 2HD ARG A 633	1.376	0.907	13.922	1.00	0.00
ATOM 1830 HE ARG A 633	1.835	3.598	15.025	1.00	0.00
ATOM 1831 IHH1 ARG A 633	-0.461	1.228	13.678	1.00	0.00
ATOM 1832 2HH1 ARG A 633	-1.857	1.932	14.423	1.00	0.00
ATOM 1833 IHH2 ARG A 633	-0.070	4.562	16.027	1.00	0.00
ATOM 1834 2HH2 ARG A 633	-1.631	3.855	15.778	1.00	0.00
ATOM 1835 N MET A 634	4.194	4.586	9.871	1.00	0.00
ATOM 1836 CA MET A 634	4.756	4.246	8.570	1.00	0.00
ATOM 1837 C MET A 634	6.239	3.832	8.629	1.00	0.00
ATOM 1838 O MET A 634	6.849	3.485	7.623	1.00	0.00
ATOM 1839 CB MET A 634	4.684	5.489	7.677	1.00	0.00
ATOM 1840 CG MET A 634	5.822	6.509	7.893	1.00	0.00
ATOM 1841 SD MET A 634	5.311	8.055	7.121	1.00	0.00
ATOM 1842 CE MET A 634	6.623	9.183	7.556	1.00	0.00
ATOM 1843 HN MET A 634	3.844	5.517	10.017	1.00	0.00
ATOM 1844 HA MET A 634	4.138	3.444	8.169	1.00	0.00
ATOM 1845 IHB MET A 634	3.717	5.974	7.823	1.00	0.00
ATOM 1846 2HB MET A 634	4.706	5.183	6.635	1.00	0.00
ATOM 1847 IHG MET A 634	6.771	6.152	7.508	1.00	0.00
ATOM 1848 2HG MET A 634	6.077	6.655	8.938	1.00	0.00
ATOM 1849 IHE MET A 634	7.173	9.429	6.652	1.00	0.00
ATOM 1850 2HE MET A 634	7.254	8.773	8.343	1.00	0.00
ATOM 1851 3HE MET A 634	6.206	10.122	7.903	1.00	0.00
ATOM 1852 N THR A 635	6.805	3.946	9.834	1.00	0.00
ATOM 1853 CA THR A 635	8.166	3.585	10.197	1.00	0.00
ATOM 1854 C THR A 635	8.562	2.126	10.015	1.00	0.00
ATOM 1855 O THR A 635	9.434	1.608	10.711	1.00	0.00
ATOM 1856 CB THR A 635	8.480	3.949	11.621	1.00	0.00
ATOM 1857 OG1 THR A 635	9.877	3.870	11.867	1.00	0.00
ATOM 1858 CG2 THR A 635	7.724	2.979	12.544	1.00	0.00
ATOM 1859 HN THR A 635	6.292	4.442	10.530	1.00	0.00
ATOM 1860 HA THR A 635	8.828	4.118	9.515	1.00	0.00
ATOM 1861 HB THR A 635	8.158	4.970	11.827	1.00	0.00

54/208

ATOM	1862	HG1 THR A 635	10.134	2.975	11.694	1.00	0.00
ATOM	1863	1HG2 THR A 635	8.151	1.978	12.483	1.00	0.00
ATOM	1864	2HG2 THR A 635	6.677	2.918	12.248	1.00	0.00
ATOM	1865	3HG2 THR A 635	7.794	3.313	13.579	1.00	0.00
ATOM	1866	N LEU A 636	7.821	1.446	9.104	1.00	0.00
ATOM	1867	CA LEU A 636	8.154	0.172	8.494	1.00	0.00
ATOM	1868	C LEU A 636	8.817	0.534	7.166	1.00	0.00
ATOM	1869	O LEU A 636	8.410	0.111	6.097	1.00	0.00
ATOM	1870	CB LEU A 636	6.897	-0.722	8.320	1.00	0.00
ATOM	1871	CG LEU A 636	5.812	-0.400	7.243	1.00	0.00
ATOM	1872	CD1 LEU A 636	5.590	1.062	6.929	1.00	0.00
ATOM	1873	CD2 LEU A 636	5.875	-1.271	5.970	1.00	0.00
ATOM	1874	HN LEU A 636	7.059	1.888	8.645	1.00	0.00
ATOM	1875	HA LEU A 636	8.869	-0.331	9.147	1.00	0.00
ATOM	1876	1HB LEU A 636	6.408	-0.765	9.294	1.00	0.00
ATOM	1877	2HB LEU A 636	7.246	-1.734	8.137	1.00	0.00
ATOM	1878	HG LEU A 636	4.857	-0.636	7.692	1.00	0.00
ATOM	1879	1HD1 LEU A 636	5.311	1.582	7.839	1.00	0.00
ATOM	1880	2HD1 LEU A 636	4.765	1.181	6.233	1.00	0.00
ATOM	1881	3HD1 LEU A 636	6.470	1.511	6.482	1.00	0.00
ATOM	1882	1HD2 LEU A 636	6.080	-2.315	6.206	1.00	0.00
ATOM	1883	2HD2 LEU A 636	6.622	-0.946	5.252	1.00	0.00
ATOM	1884	3HD2 LEU A 636	4.921	-1.241	5.443	1.00	0.00
ATOM	1885	N PRO A 637	9.812	1.437	7.273	1.00	0.00
ATOM	1886	CA PRO A 637	10.350	2.125	6.111	1.00	0.00
ATOM	1887	C PRO A 637	10.363	1.662	4.692	1.00	0.00
ATOM	1888	O PRO A 637	10.335	0.477	4.364	1.00	0.00
ATOM	1889	CB PRO A 637	11.736	2.648	6.492	1.00	0.00
ATOM	1890	CG PRO A 637	12.187	1.711	7.606	1.00	0.00
ATOM	1891	CD PRO A 637	10.867	1.322	8.280	1.00	0.00
ATOM	1892	1HD PRO A 637	10.912	0.298	8.651	1.00	0.00
ATOM	1893	2HD PRO A 637	10.651	1.989	9.115	1.00	0.00
ATOM	1894	HA PRO A 637	9.692	2.949	5.834	1.00	0.00
ATOM	1895	1HB PRO A 637	11.685	3.679	6.841	1.00	0.00
ATOM	1896	2HB PRO A 637	12.419	2.609	5.643	1.00	0.00
ATOM	1897	1HG PRO A 637	12.702	0.837	7.207	1.00	0.00
ATOM	1898	2HG PRO A 637	12.857	2.214	8.303	1.00	0.00
ATOM	1899	N CYS A 638	10.449	2.743	3.865	1.00	0.00
ATOM	1900	CA CYS A 638	10.294	2.855	2.427	1.00	0.00
ATOM	1901	C CYS A 638	8.818	3.110	2.059	1.00	0.00
ATOM	1902	O CYS A 638	8.523	3.510	0.936	1.00	0.00
ATOM	1903	CB CYS A 638	10.982	1.745	1.628	1.00	0.00
ATOM	1904	SG CYS A 638	10.969	2.069	-0.161	1.00	0.00
ATOM	1905	HN CYS A 638	10.630	3.611	4.327	1.00	0.00
ATOM	1906	HA CYS A 638	10.814	3.783	2.192	1.00	0.00
ATOM	1907	1HB CYS A 638	10.524	0.785	1.832	1.00	0.00
ATOM	1908	2HB CYS A 638	12.019	1.656	1.951	1.00	0.00
ATOM	1909	HG CYS A 638	11.560	1.050	-0.793	1.00	0.00
ATOM	1910	N MET A 639	7.943	2.913	3.080	1.00	0.00



55/208

ATOM 1911 CA MET A 639	6.573	3.419	3.022	1.00	0.00
ATOM 1912 C MET A 639	6.516	4.893	3.449	1.00	0.00
ATOM 1913 O MET A 639	5.612	5.614	3.065	1.00	0.00
ATOM 1914 CB MET A 639	5.630	2.616	3.935	1.00	0.00
ATOM 1915 CG MET A 639	4.149	2.912	3.646	1.00	0.00
ATOM 1916 SD MET A 639	3.022	1.729	4.408	1.00	0.00
ATOM 1917 CE MET A 639	2.363	2.759	5.733	1.00	0.00
ATOM 1918 HN MET A 639	8.222	2.383	3.879	1.00	0.00
ATOM 1919 HA MET A 639	6.243	3.341	1.983	1.00	0.00
ATOM 1920 IHB MET A 639	5.842	2.853	4.976	1.00	0.00
ATOM 1921 2HB MET A 639	5.812	1.549	3.817	1.00	0.00
ATOM 1922 IHG MET A 639	3.991	2.853	2.574	1.00	0.00
ATOM 1923 2HG MET A 639	3.875	3.928	3.931	1.00	0.00
ATOM 1924 IHE MET A 639	2.035	2.132	6.563	1.00	0.00
ATOM 1925 2HE MET A 639	1.522	3.354	5.376	1.00	0.00
ATOM 1926 3HE MET A 639	3.133	3.427	6.113	1.00	0.00
ATOM 1927 N TYR A 640	7.505	5.290	4.280	1.00	0.00
ATOM 1928 CA TYR A 640	7.618	6.639	4.842	1.00	0.00
ATOM 1929 C TYR A 640	7.155	7.706	3.865	1.00	0.00
ATOM 1930 O TYR A 640	6.223	8.472	4.087	1.00	0.00
ATOM 1931 CB TYR A 640	9.112	6.859	5.261	1.00	0.00
ATOM 1932 CG TYR A 640	9.494	8.274	5.672	1.00	0.00
ATOM 1933 CD1 TYR A 640	9.735	9.264	4.719	1.00	0.00
ATOM 1934 CD2 TYR A 640	9.594	8.630	7.016	1.00	0.00
ATOM 1935 CE1 TYR A 640	9.961	10.583	5.086	1.00	0.00
ATOM 1936 CE2 TYR A 640	9.828	9.953	7.392	1.00	0.00
ATOM 1937 CZ TYR A 640	9.977	10.941	6.424	1.00	0.00
ATOM 1938 OH TYR A 640	10.117	12.278	6.766	1.00	0.00
ATOM 1939 HN TYR A 640	8.092	4.572	4.641	1.00	0.00
ATOM 1940 HA TYR A 640	6.931	6.686	5.661	1.00	0.00
ATOM 1941 IHB TYR A 640	9.768	6.572	4.439	1.00	0.00
ATOM 1942 2HB TYR A 640	9.355	6.179	6.079	1.00	0.00
ATOM 1943 HD1 TYR A 640	9.757	9.027	3.668	1.00	0.00
ATOM 1944 HE1 TYR A 640	10.124	11.326	4.321	1.00	0.00
ATOM 1945 HD2 TYR A 640	9.464	7.879	7.782	1.00	0.00
ATOM 1946 HE2 TYR A 640	9.866	10.198	8.444	1.00	0.00
ATOM 1947 HH TYR A 640	10.860	12.349	7.362	1.00	0.00
ATOM 1948 N ASP A 641	7.900	7.689	2.756	1.00	0.00
ATOM 1949 CA ASP A 641	7.691	8.725	1.788	1.00	0.00
ATOM 1950 C ASP A 641	6.322	8.607	1.202	1.00	0.00
ATOM 1951 O ASP A 641	5.659	9.612	0.950	1.00	0.00
ATOM 1952 CB ASP A 641	8.725	8.718	0.644	1.00	0.00
ATOM 1953 CG ASP A 641	8.628	7.412	-0.130	1.00	0.00
ATOM 1954 OD1 ASP A 641	8.232	6.383	0.482	1.00	0.00
ATOM 1955 OD2 ASP A 641	8.951	7.425	-1.348	1.00	0.00
ATOM 1956 HN ASP A 641	8.594	6.986	2.603	1.00	0.00
ATOM 1957 HA ASP A 641	7.744	9.669	2.330	1.00	0.00
ATOM 1958 IHB ASP A 641	9.732	8.812	1.049	1.00	0.00
ATOM 1959 2HB ASP A 641	8.535	9.546	-0.038	1.00	0.00

56/208

ATOM	1960	N	GLN A 642	5.820	7.376	0.975	1.00	0.00
ATOM	1961	CA	GLN A 642	4.539	7.246	0.288	1.00	0.00
ATOM	1962	C	GLN A 642	3.405	7.741	1.196	1.00	0.00
ATOM	1963	O	GLN A 642	2.481	8.398	0.744	1.00	0.00
ATOM	1964	CB	GLN A 642	4.351	5.846	-0.336	1.00	0.00
ATOM	1965	CG	GLN A 642	3.695	4.769	0.544	1.00	0.00
ATOM	1966	CD	GLN A 642	2.169	4.926	0.592	1.00	0.00
ATOM	1967	OE1	GLN A 642	1.499	4.941	-0.429	1.00	0.00
ATOM	1968	NE2	GLN A 642	1.658	5.033	1.823	1.00	0.00
ATOM	1969	HN	GLN A 642	6.396	6.590	1.211	1.00	0.00
ATOM	1970	HA	GLN A 642	4.591	7.947	-0.548	1.00	0.00
ATOM	1971	1HB	GLN A 642	5.329	5.487	-0.658	1.00	0.00
ATOM	1972	2HB	GLN A 642	3.771	5.944	-1.256	1.00	0.00
ATOM	1973	1HG	GLN A 642	4.104	4.785	1.547	1.00	0.00
ATOM	1974	2HG	GLN A 642	3.903	3.782	0.131	1.00	0.00
ATOM	1975	1HE2	GLN A 642	2.223	5.000	2.645	1.00	0.00
ATOM	1976	2HE2	GLN A 642	0.669	5.157	1.891	1.00	0.00
ATOM	1977	N	CYS A 643	3.555	7.450	2.506	1.00	0.00
ATOM	1978	CA	CYS A 643	2.631	8.001	3.484	1.00	0.00
ATOM	1979	C	CYS A 643	2.626	9.534	3.413	1.00	0.00
ATOM	1980	O	CYS A 643	1.580	10.157	3.530	1.00	0.00
ATOM	1981	CB	CYS A 643	3.045	7.537	4.885	1.00	0.00
ATOM	1982	SG	CYS A 643	2.794	8.786	6.171	1.00	0.00
ATOM	1983	HN	CYS A 643	4.332	6.879	2.775	1.00	0.00
ATOM	1984	HA	CYS A 643	1.634	7.633	3.235	1.00	0.00
ATOM	1985	1HB	CYS A 643	4.097	7.254	4.889	1.00	0.00
ATOM	1986	2HB	CYS A 643	2.489	6.639	5.154	1.00	0.00
ATOM	1987	HG	CYS A 643	2.847	8.193	7.368	1.00	0.00
ATOM	1988	N	LYS A 644	3.835	10.104	3.196	1.00	0.00
ATOM	1989	CA	LYS A 644	3.964	11.530	3.171	1.00	0.00
ATOM	1990	C	LYS A 644	3.198	12.069	2.014	1.00	0.00
ATOM	1991	O	LYS A 644	2.389	12.983	2.164	1.00	0.00
ATOM	1992	CB	LYS A 644	5.421	11.993	2.987	1.00	0.00
ATOM	1993	CG	LYS A 644	6.299	11.902	4.238	1.00	0.00
ATOM	1994	CD	LYS A 644	5.885	12.868	5.350	1.00	0.00
ATOM	1995	CE	LYS A 644	6.921	12.991	6.470	1.00	0.00
ATOM	1996	NZ	LYS A 644	8.145	13.645	5.957	1.00	0.00
ATOM	1997	HN	LYS A 644	4.648	9.527	3.117	1.00	0.00
ATOM	1998	HA	LYS A 644	3.570	11.896	4.118	1.00	0.00
ATOM	1999	1HB	LYS A 644	5.409	13.030	2.655	1.00	0.00
ATOM	2000	2HB	LYS A 644	5.876	11.387	2.206	1.00	0.00
ATOM	2001	1HG	LYS A 644	7.330	12.114	3.957	1.00	0.00
ATOM	2002	2HG	LYS A 644	6.251	10.884	4.624	1.00	0.00
ATOM	2003	1HD	LYS A 644	4.945	12.525	5.780	1.00	0.00
ATOM	2004	2HD	LYS A 644	5.722	13.853	4.914	1.00	0.00
ATOM	2005	1HE	LYS A 644	7.194	12.005	6.844	1.00	0.00
ATOM	2006	2HE	LYS A 644	6.528	13.597	7.286	1.00	0.00
ATOM	2007	1HZ	LYS A 644	7.909	14.595	5.604	1.00	0.00
ATOM	2008	2HZ	LYS A 644	8.544	13.077	5.183	1.00	0.00

57/208

ATOM 2009 3HZ LYS A 644	8.843	13.725	6.724	1.00	0.00
ATOM 2010 N HIS A 645	3.413	11.483	0.825	1.00	0.00
ATOM 2011 CA HIS A 645	2.750	11.978	-0.342	1.00	0.00
ATOM 2012 C HIS A 645	1.281	11.777	-0.183	1.00	0.00
ATOM 2013 O HIS A 645	0.485	12.612	-0.611	1.00	0.00
ATOM 2014 CB HIS A 645	3.245	11.314	-1.636	1.00	0.00
ATOM 2015 CG HIS A 645	4.645	11.751	-1.963	1.00	0.00
ATOM 2016 ND1 HIS A 645	5.461	11.146	-2.893	1.00	0.00
ATOM 2017 CD2 HIS A 645	5.363	12.796	-1.465	1.00	0.00
ATOM 2018 CE1 HIS A 645	6.623	11.848	-2.909	1.00	0.00
ATOM 2019 NE2 HIS A 645	6.610	12.858	-2.059	1.00	0.00
ATOM 2020 HN HIS A 645	4.035	10.704	0.756	1.00	0.00
ATOM 2021 HA HIS A 645	2.938	13.051	-0.376	1.00	0.00
ATOM 2022 1HB HIS A 645	2.590	11.588	-2.463	1.00	0.00
ATOM 2023 2HB HIS A 645	3.234	10.231	-1.521	1.00	0.00
ATOM 2024 HD2 HIS A 645	5.007	13.481	-0.711	1.00	0.00
ATOM 2025 HD1 HIS A 645	5.244	10.361	-3.438	1.00	0.00
ATOM 2026 HE1 HIS A 645	7.462	11.607	-3.544	1.00	0.00
ATOM 2027 N MET A 646	0.886	10.654	0.460	1.00	0.00
ATOM 2028 CA MET A 646	-0.539	10.371	0.669	1.00	0.00
ATOM 2029 C MET A 646	-1.199	11.378	1.633	1.00	0.00
ATOM 2030 O MET A 646	-2.362	11.742	1.495	1.00	0.00
ATOM 2031 CB MET A 646	-0.755	8.943	1.199	1.00	0.00
ATOM 2032 CG MET A 646	-0.620	7.867	0.116	1.00	0.00
ATOM 2033 SD MET A 646	-1.146	6.270	0.769	1.00	0.00
ATOM 2034 CE MET A 646	-2.105	5.669	-0.634	1.00	0.00
ATOM 2035 HN MET A 646	1.576	9.999	0.768	1.00	0.00
ATOM 2036 HA MET A 646	-1.022	10.471	-0.303	1.00	0.00
ATOM 2037 1HB MET A 646	-1.763	8.859	1.610	1.00	0.00
ATOM 2038 2HB MET A 646	-0.075	8.738	2.027	1.00	0.00
ATOM 2039 1HG MET A 646	0.406	7.791	-0.241	1.00	0.00
ATOM 2040 2HG MET A 646	-1.243	8.141	-0.735	1.00	0.00
ATOM 2041 1HE MET A 646	-2.864	4.977	-0.275	1.00	0.00
ATOM 2042 2HE MET A 646	-1.459	5.169	-1.356	1.00	0.00
ATOM 2043 3HE MET A 646	-2.632	6.484	-1.129	1.00	0.00
ATOM 2044 N LEU A 647	-0.416	11.831	2.622	1.00	0.00
ATOM 2045 CA LEU A 647	-0.963	12.840	3.484	1.00	0.00
ATOM 2046 C LEU A 647	-1.102	14.128	2.759	1.00	0.00
ATOM 2047 O LEU A 647	-2.124	14.808	2.872	1.00	0.00
ATOM 2048 CB LEU A 647	-0.078	13.164	4.691	1.00	0.00
ATOM 2049 CG LEU A 647	-0.153	12.091	5.768	1.00	0.00
ATOM 2050 CD1 LEU A 647	0.730	12.449	6.975	1.00	0.00
ATOM 2051 CD2 LEU A 647	-1.626	11.821	6.118	1.00	0.00
ATOM 2052 HN LEU A 647	0.457	11.394	2.840	1.00	0.00
ATOM 2053 HA LEU A 647	-1.929	12.466	3.822	1.00	0.00
ATOM 2054 1HB LEU A 647	-0.393	14.116	5.117	1.00	0.00
ATOM 2055 2HB LEU A 647	0.955	13.262	4.359	1.00	0.00
ATOM 2056 HG LEU A 647	0.175	11.139	5.351	1.00	0.00
ATOM 2057 1HD1 LEU A 647	0.117	12.701	7.840	1.00	0.00

58/208

ATOM	2058	2HD1	LEU	A 647	1.354	13.312	6.741	1.00	0.00
ATOM	2059	3HD1	LEU	A 647	1.361	11.602	7.244	1.00	0.00
ATOM	2060	1HD2	LEU	A 647	-2.243	11.826	5.219	1.00	0.00
ATOM	2061	2HD2	LEU	A 647	-2.002	12.594	6.788	1.00	0.00
ATOM	2062	3HD2	LEU	A 647	-1.728	10.844	6.591	1.00	0.00
ATOM	2063	N	TYR	A 648	-0.080	14.492	1.971	1.00	0.00
ATOM	2064	CA	TYR	A 648	-0.102	15.769	1.332	1.00	0.00
ATOM	2065	C	TYR	A 648	-1.285	15.860	0.425	1.00	0.00
ATOM	2066	O	TYR	A 648	-1.946	16.896	0.366	1.00	0.00
ATOM	2067	CB	TYR	A 648	1.167	16.042	0.507	1.00	0.00
ATOM	2068	CG	TYR	A 648	1.014	17.399	-0.087	1.00	0.00
ATOM	2069	CD1	TYR	A 648	0.389	17.572	-1.299	1.00	0.00
ATOM	2070	CD2	TYR	A 648	1.439	18.507	0.610	1.00	0.00
ATOM	2071	CE1	TYR	A 648	0.206	18.831	-1.817	1.00	0.00
ATOM	2072	CE2	TYR	A 648	1.257	19.769	0.098	1.00	0.00
ATOM	2073	CZ	TYR	A 648	0.640	19.932	-1.118	1.00	0.00
ATOM	2074	OH	TYR	A 648	0.444	21.226	-1.644	1.00	0.00
ATOM	2075	HN	TYR	A 648	0.692	13.872	1.832	1.00	0.00
ATOM	2076	HA	TYR	A 648	-0.202	16.513	2.123	1.00	0.00
ATOM	2077	1HB	TYR	A 648	1.277	15.303	-0.286	1.00	0.00
ATOM	2078	2HB	TYR	A 648	2.053	16.014	1.141	1.00	0.00
ATOM	2079	HD1	TYR	A 648	0.038	16.711	-1.849	1.00	0.00
ATOM	2080	HE1	TYR	A 648	-0.278	18.956	-2.774	1.00	0.00
ATOM	2081	HD2	TYR	A 648	1.921	18.383	1.569	1.00	0.00
ATOM	2082	HE2	TYR	A 648	1.599	20.631	0.652	1.00	0.00
ATOM	2083	HH	TYR	A 648	-0.245	21.202	-2.295	1.00	0.00
ATOM	2084	N	VAL	A 649	-1.593	14.783	-0.320	1.00	0.00
ATOM	2085	CA	VAL	A 649	-2.721	14.865	-1.204	1.00	0.00
ATOM	2086	C	VAL	A 649	-3.964	14.983	-0.384	1.00	0.00
ATOM	2087	O	VAL	A 649	-4.867	15.755	-0.707	1.00	0.00
ATOM	2088	CB	VAL	A 649	-2.861	13.681	-2.118	1.00	0.00
ATOM	2089	CG1	VAL	A 649	-3.212	12.435	-1.292	1.00	0.00
ATOM	2090	CG2	VAL	A 649	-3.907	14.026	-3.193	1.00	0.00
ATOM	2091	HN	VAL	A 649	-1.049	13.946	-0.260	1.00	0.00
ATOM	2092	HA	VAL	A 649	-2.586	15.773	-1.791	1.00	0.00
ATOM	2093	HB	VAL	A 649	-1.927	13.516	-2.655	1.00	0.00
ATOM	2094	1HG1	VAL	A 649	-4.048	12.639	-0.623	1.00	0.00
ATOM	2095	2HG1	VAL	A 649	-2.359	12.135	-0.683	1.00	0.00
ATOM	2096	3HG1	VAL	A 649	-3.499	11.615	-1.950	1.00	0.00
ATOM	2097	1HG2	VAL	A 649	-3.686	14.991	-3.650	1.00	0.00
ATOM	2098	2HG2	VAL	A 649	-4.900	14.084	-2.747	1.00	0.00
ATOM	2099	3HG2	VAL	A 649	-3.902	13.272	-3.979	1.00	0.00
ATOM	2100	N	SER	A 650	-4.023	14.232	0.732	1.00	0.00
ATOM	2101	CA	SER	A 650	-5.193	14.243	1.556	1.00	0.00
ATOM	2102	C	SER	A 650	-5.420	15.645	2.021	1.00	0.00
ATOM	2103	O	SER	A 650	-6.549	16.135	2.029	1.00	0.00
ATOM	2104	CB	SER	A 650	-5.044	13.361	2.807	1.00	0.00
ATOM	2105	OG	SER	A 650	-6.232	13.412	3.584	1.00	0.00
ATOM	2106	HN	SER	A 650	-3.241	13.662	0.986	1.00	0.00

59/208

ATOM 2107 HA SER A 650	-6.015	13.884	0.938	1.00	0.00
ATOM 2108 IHB SER A 650	-4.217	13.714	3.423	1.00	0.00
ATOM 2109 2HB SER A 650	-4.869	12.324	2.520	1.00	0.00
ATOM 2110 HG SER A 650	-6.530	14.312	3.566	1.00	0.00
ATOM 2111 N SER A 651	-4.335	16.334	2.416	1.00	0.00
ATOM 2112 CA SER A 651	-4.456	17.677	2.903	1.00	0.00
ATOM 2113 C SER A 651	-4.931	18.597	1.820	1.00	0.00
ATOM 2114 O SER A 651	-5.771	19.464	2.059	1.00	0.00
ATOM 2115 CB SER A 651	-3.139	18.242	3.471	1.00	0.00
ATOM 2116 OG SER A 651	-2.170	18.402	2.446	1.00	0.00
ATOM 2117 HN SER A 651	-3.434	15.904	2.369	1.00	0.00
ATOM 2118 HA SER A 651	-5.219	17.657	3.680	1.00	0.00
ATOM 2119 IHB SER A 651	-2.732	17.561	4.218	1.00	0.00
ATOM 2120 2HB SER A 651	-3.315	19.218	3.924	1.00	0.00
ATOM 2121 HG SER A 651	-2.577	18.115	1.639	1.00	0.00
ATOM 2122 N GLU A 652	-4.421	18.421	0.586	1.00	0.00
ATOM 2123 CA GLU A 652	-4.800	19.296	-0.486	1.00	0.00
ATOM 2124 C GLU A 652	-6.268	19.145	-0.716	1.00	0.00
ATOM 2125 O GLU A 652	-6.970	20.122	-0.969	1.00	0.00
ATOM 2126 CB GLU A 652	-4.057	18.993	-1.797	1.00	0.00
ATOM 2127 CG GLU A 652	-4.250	20.074	-2.862	1.00	0.00
ATOM 2128 CD GLU A 652	-3.249	19.813	-3.976	1.00	0.00
ATOM 2129 OE1 GLU A 652	-2.042	19.647	-3.657	1.00	0.00
ATOM 2130 OE2 GLU A 652	-3.677	19.773	-5.160	1.00	0.00
ATOM 2131 HN GLU A 652	-3.774	17.677	0.417	1.00	0.00
ATOM 2132 HA GLU A 652	-4.576	20.310	-0.154	1.00	0.00
ATOM 2133 IHB GLU A 652	-4.416	18.044	-2.192	1.00	0.00
ATOM 2134 2HB GLU A 652	-2.994	18.897	-1.584	1.00	0.00
ATOM 2135 IHG GLU A 652	-4.072	21.063	-2.441	1.00	0.00
ATOM 2136 2HG GLU A 652	-5.261	20.036	-3.268	1.00	0.00
ATOM 2137 N LEU A 653	-6.779	17.906	-0.610	1.00	0.00
ATOM 2138 CA LEU A 653	-8.176	17.673	-0.822	1.00	0.00
ATOM 2139 C LEU A 653	-8.916	18.459	0.215	1.00	0.00
ATOM 2140 O LEU A 653	-9.976	19.020	-0.063	1.00	0.00
ATOM 2141 CB LEU A 653	-8.555	16.191	-0.658	1.00	0.00
ATOM 2142 CG LEU A 653	-7.855	15.278	-1.684	1.00	0.00
ATOM 2143 CD1 LEU A 653	-8.258	13.807	-1.496	1.00	0.00
ATOM 2144 CD2 LEU A 653	-8.074	15.782	-3.118	1.00	0.00
ATOM 2145 HN LEU A 653	-6.177	17.141	-0.381	1.00	0.00
ATOM 2146 HA LEU A 653	-8.401	18.010	-1.834	1.00	0.00
ATOM 2147 IHB LEU A 653	-9.633	16.088	-0.772	1.00	0.00
ATOM 2148 2HB LEU A 653	-8.284	15.867	0.346	1.00	0.00
ATOM 2149 HG LEU A 653	-6.775	15.372	-1.571	1.00	0.00
ATOM 2150 IHD1 LEU A 653	-9.334	13.684	-1.619	1.00	0.00
ATOM 2151 2HD1 LEU A 653	-7.994	13.469	-0.494	1.00	0.00
ATOM 2152 3HD1 LEU A 653	-7.760	13.182	-2.237	1.00	0.00
ATOM 2153 1HD2 LEU A 653	-7.394	16.603	-3.347	1.00	0.00
ATOM 2154 2HD2 LEU A 653	-9.094	16.147	-3.238	1.00	0.00
ATOM 2155 3HD2 LEU A 653	-7.885	14.980	-3.832	1.00	0.00

60/208

ATOM	2156	N	HIS A 654	-8.355	18.527	1.440	1.00	0.00
ATOM	2157	CA	HIS A 654	-8.965	19.245	2.528	1.00	0.00
ATOM	2158	C	HIS A 654	-9.167	20.664	2.111	1.00	0.00
ATOM	2159	O	HIS A 654	-10.270	21.201	2.179	1.00	0.00
ATOM	2160	CB	HIS A 654	-8.019	19.455	3.728	1.00	0.00
ATOM	2161	CG	HIS A 654	-7.730	18.335	4.681	1.00	0.00
ATOM	2162	ND1	HIS A 654	-8.058	18.419	6.018	1.00	0.00
ATOM	2163	CD2	HIS A 654	-6.904	17.262	4.569	1.00	0.00
ATOM	2164	CE1	HIS A 654	-7.416	17.402	6.643	1.00	0.00
ATOM	2165	NE2	HIS A 654	-6.709	16.666	5.803	1.00	0.00
ATOM	2166	HN	HIS A 654	-7.485	18.062	1.597	1.00	0.00
ATOM	2167	HA	HIS A 654	-9.834	18.662	2.835	1.00	0.00
ATOM	2168	1HB	HIS A 654	-8.436	20.261	4.326	1.00	0.00
ATOM	2169	2HB	HIS A 654	-7.058	19.766	3.327	1.00	0.00
ATOM	2170	HD2	HIS A 654	-6.461	16.921	3.645	1.00	0.00
ATOM	2171	HD1	HIS A 654	-8.643	19.085	6.435	1.00	0.00
ATOM	2172	HE1	HIS A 654	-7.476	17.215	7.704	1.00	0.00
ATOM	2173	N	ARG A 655	-8.078	21.301	1.645	1.00	0.00
ATOM	2174	CA	ARG A 655	-8.117	22.702	1.345	1.00	0.00
ATOM	2175	C	ARG A 655	-9.090	23.001	0.254	1.00	0.00
ATOM	2176	O	ARG A 655	-9.843	23.970	0.334	1.00	0.00
ATOM	2177	CB	ARG A 655	-6.736	23.261	0.961	1.00	0.00
ATOM	2178	CG	ARG A 655	-5.822	23.434	2.179	1.00	0.00
ATOM	2179	CD	ARG A 655	-5.468	22.124	2.888	1.00	0.00
ATOM	2180	NE	ARG A 655	-4.054	21.795	2.558	1.00	0.00
ATOM	2181	CZ	ARG A 655	-3.045	22.307	3.323	1.00	0.00
ATOM	2182	NH1	ARG A 655	-3.338	23.121	4.379	1.00	0.00
ATOM	2183	NH2	ARG A 655	-1.746	22.004	3.036	1.00	0.00
ATOM	2184	HN	ARG A 655	-7.230	20.790	1.506	1.00	0.00
ATOM	2185	HA	ARG A 655	-8.490	23.203	2.238	1.00	0.00
ATOM	2186	1HB	ARG A 655	-6.866	24.226	0.473	1.00	0.00
ATOM	2187	2HB	ARG A 655	-6.261	22.582	0.253	1.00	0.00
ATOM	2188	1HG	ARG A 655	-6.317	24.092	2.892	1.00	0.00
ATOM	2189	2HG	ARG A 655	-4.899	23.913	1.854	1.00	0.00
ATOM	2190	1HD	ARG A 655	-6.094	21.304	2.539	1.00	0.00
ATOM	2191	2HD	ARG A 655	-5.545	22.228	3.970	1.00	0.00
ATOM	2192	HE	ARG A 655	-3.843	21.202	1.781	1.00	0.00
ATOM	2193	1HH1	ARG A 655	-4.290	23.341	4.591	1.00	0.00
ATOM	2194	2HH1	ARG A 655	-2.601	23.497	4.940	1.00	0.00
ATOM	2195	1HH2	ARG A 655	-1.531	21.406	2.264	1.00	0.00
ATOM	2196	2HH2	ARG A 655	-1.009	22.380	3.598	1.00	0.00
ATOM	2197	N	LEU A 656	-9.103	22.163	-0.792	1.00	0.00
ATOM	2198	CA	LEU A 656	-10.001	22.337	-1.896	1.00	0.00
ATOM	2199	C	LEU A 656	-11.407	22.100	-1.453	1.00	0.00
ATOM	2200	O	LEU A 656	-12.349	22.583	-2.080	1.00	0.00
ATOM	2201	CB	LEU A 656	-9.700	21.407	-3.087	1.00	0.00
ATOM	2202	CG	LEU A 656	-8.472	21.835	-3.918	1.00	0.00
ATOM	2203	CD1	LEU A 656	-7.183	21.850	-3.084	1.00	0.00
ATOM	2204	CD2	LEU A 656	-8.342	20.980	-5.189	1.00	0.00

61/208

ATOM	2205	HN	LEU	A	656	-8.466	21.392	-0.802	1.00	0.00
ATOM	2206	HA	LEU	A	656	-9.912	23.378	-2.205	1.00	0.00
ATOM	2207	1HB	LEU	A	656	-10.572	21.386	-3.740	1.00	0.00
ATOM	2208	2HB	LEU	A	656	-9.531	20.400	-2.709	1.00	0.00
ATOM	2209	HG	LEU	A	656	-8.646	22.832	-4.322	1.00	0.00
ATOM	2210	1HD1	LEU	A	656	-6.878	20.835	-2.827	1.00	0.00
ATOM	2211	2HD1	LEU	A	656	-7.341	22.399	-2.156	1.00	0.00
ATOM	2212	3HD1	LEU	A	656	-6.374	22.311	-3.650	1.00	0.00
ATOM	2213	1HD2	LEU	A	656	-9.227	21.085	-5.816	1.00	0.00
ATOM	2214	2HD2	LEU	A	656	-8.238	19.928	-4.926	1.00	0.00
ATOM	2215	3HD2	LEU	A	656	-7.477	21.300	-5.771	1.00	0.00
ATOM	2216	N	GLN	A	657	-11.597	21.333	-0.364	1.00	0.00
ATOM	2217	CA	GLN	A	657	-12.934	21.062	0.071	1.00	0.00
ATOM	2218	C	GLN	A	657	-13.598	20.292	-1.019	1.00	0.00
ATOM	2219	O	GLN	A	657	-14.683	20.641	-1.479	1.00	0.00
ATOM	2220	CB	GLN	A	657	-13.761	22.338	0.306	1.00	0.00
ATOM	2221	CG	GLN	A	657	-13.224	23.227	1.431	1.00	0.00
ATOM	2222	CD	GLN	A	657	-14.135	24.442	1.541	1.00	0.00
ATOM	2223	OE1	GLN	A	657	-13.875	25.359	2.318	1.00	0.00
ATOM	2224	NE2	GLN	A	657	-15.231	24.454	0.738	1.00	0.00
ATOM	2225	HN	GLN	A	657	-10.815	20.957	0.134	1.00	0.00
ATOM	2226	HA	GLN	A	657	-12.851	20.493	0.997	1.00	0.00
ATOM	2227	1HB	GLN	A	657	-14.783	22.051	0.549	1.00	0.00
ATOM	2228	2HB	GLN	A	657	-13.777	22.917	-0.616	1.00	0.00
ATOM	2229	1HG	GLN	A	657	-12.209	23.556	1.208	1.00	0.00
ATOM	2230	2HG	GLN	A	657	-13.224	22.688	2.378	1.00	0.00
ATOM	2231	1HE2	GLN	A	657	-15.938	25.149	0.875	1.00	0.00
ATOM	2232	2HE2	GLN	A	657	-15.347	23.780	0.009	1.00	0.00
ATOM	2233	N	VAL	A	658	-12.935	19.205	-1.457	1.00	0.00
ATOM	2234	CA	VAL	A	658	-13.459	18.405	-2.523	1.00	0.00
ATOM	2235	C	VAL	A	658	-14.729	17.748	-2.099	1.00	0.00
ATOM	2236	O	VAL	A	658	-14.827	17.196	-1.003	1.00	0.00
ATOM	2237	CB	VAL	A	658	-12.516	17.329	-2.978	1.00	0.00
ATOM	2238	CG1	VAL	A	658	-11.249	17.994	-3.543	1.00	0.00
ATOM	2239	CG2	VAL	A	658	-12.249	16.381	-1.797	1.00	0.00
ATOM	2240	HN	VAL	A	658	-12.065	18.954	-1.033	1.00	0.00
ATOM	2241	HA	VAL	A	658	-13.671	19.087	-3.346	1.00	0.00
ATOM	2242	HB	VAL	A	658	-12.991	16.718	-3.746	1.00	0.00
ATOM	2243	1HG1	VAL	A	658	-10.668	18.456	-2.745	1.00	0.00
ATOM	2244	2HG1	VAL	A	658	-11.519	18.772	-4.257	1.00	0.00
ATOM	2245	3HG1	VAL	A	658	-10.620	17.250	-4.032	1.00	0.00
ATOM	2246	1HG2	VAL	A	658	-13.032	16.474	-1.044	1.00	0.00
ATOM	2247	2HG2	VAL	A	658	-11.298	16.627	-1.325	1.00	0.00
ATOM	2248	3HG2	VAL	A	658	-12.232	15.347	-2.140	1.00	0.00
ATOM	2249	N	SER	A	659	-15.746	17.803	-2.984	1.00	0.00
ATOM	2250	CA	SER	A	659	-17.023	17.228	-2.686	1.00	0.00
ATOM	2251	C	SER	A	659	-17.056	15.801	-3.130	1.00	0.00
ATOM	2252	O	SER	A	659	-16.241	15.359	-3.938	1.00	0.00
ATOM	2253	CB	SER	A	659	-18.205	17.959	-3.344	1.00	0.00

62/208

ATOM	2254	OG	SER A 659	-18.194	17.764	-4.749	1.00	0.00
ATOM	2255	HN	SER A 659	-15.604	18.255	-3.864	1.00	0.00
ATOM	2256	HA	SER A 659	-17.128	17.258	-1.601	1.00	0.00
ATOM	2257	IHB	SER A 659	-18.140	19.029	-3.150	1.00	0.00
ATOM	2258	2HB	SER A 659	-19.148	17.574	-2.956	1.00	0.00
ATOM	2259	HG	SER A 659	-18.584	18.538	-5.134	1.00	0.00
ATOM	2260	N	TYR A 660	-18.026	15.044	-2.584	1.00	0.00
ATOM	2261	CA	TYR A 660	-18.187	13.647	-2.862	1.00	0.00
ATOM	2262	C	TYR A 660	-18.532	13.452	-4.305	1.00	0.00
ATOM	2263	O	TYR A 660	-18.025	12.539	-4.953	1.00	0.00
ATOM	2264	CB	TYR A 660	-19.292	13.024	-1.984	1.00	0.00
ATOM	2265	CG	TYR A 660	-19.424	11.571	-2.291	1.00	0.00
ATOM	2266	CD1	TYR A 660	-20.300	11.128	-3.255	1.00	0.00
ATOM	2267	CD2	TYR A 660	-18.694	10.647	-1.579	1.00	0.00
ATOM	2268	CE1	TYR A 660	-20.449	9.782	-3.499	1.00	0.00
ATOM	2269	CE2	TYR A 660	-18.824	9.301	-1.832	1.00	0.00
ATOM	2270	CZ	TYR A 660	-19.704	8.867	-2.793	1.00	0.00
ATOM	2271	OH	TYR A 660	-19.835	7.489	-3.061	1.00	0.00
ATOM	2272	HN	TYR A 660	-18.666	15.479	-1.952	1.00	0.00
ATOM	2273	HA	TYR A 660	-17.228	13.169	-2.663	1.00	0.00
ATOM	2274	IHB	TYR A 660	-20.245	13.517	-2.179	1.00	0.00
ATOM	2275	2HB	TYR A 660	-19.043	13.144	-0.930	1.00	0.00
ATOM	2276	HD1	TYR A 660	-20.875	11.842	-3.826	1.00	0.00
ATOM	2277	HE1	TYR A 660	-21.152	9.443	-4.245	1.00	0.00
ATOM	2278	HD2	TYR A 660	-18.011	10.982	-0.812	1.00	0.00
ATOM	2279	HE2	TYR A 660	-18.235	8.587	-1.275	1.00	0.00
ATOM	2280	HH	TYR A 660	-19.330	7.267	-3.832	1.00	0.00
ATOM	2281	N	GLU A 661	-19.398	14.316	-4.864	1.00	0.00
ATOM	2282	CA	GLU A 661	-19.761	14.171	-6.244	1.00	0.00
ATOM	2283	C	GLU A 661	-18.536	14.346	-7.089	1.00	0.00
ATOM	2284	O	GLU A 661	-18.372	13.667	-8.103	1.00	0.00
ATOM	2285	CB	GLU A 661	-20.863	15.156	-6.680	1.00	0.00
ATOM	2286	CG	GLU A 661	-20.651	16.585	-6.182	1.00	0.00
ATOM	2287	CD	GLU A 661	-21.158	16.652	-4.749	1.00	0.00
ATOM	2288	OE1	GLU A 661	-20.840	17.652	-4.055	1.00	0.00
ATOM	2289	OE2	GLU A 661	-21.873	15.702	-4.330	1.00	0.00
ATOM	2290	HN	GLU A 661	-19.787	15.057	-4.317	1.00	0.00
ATOM	2291	HA	GLU A 661	-20.104	13.145	-6.370	1.00	0.00
ATOM	2292	IHB	GLU A 661	-21.819	14.796	-6.303	1.00	0.00
ATOM	2293	2HB	GLU A 661	-20.906	15.170	-7.768	1.00	0.00
ATOM	2294	IHG	GLU A 661	-21.206	17.293	-6.797	1.00	0.00
ATOM	2295	2HG	GLU A 661	-19.593	16.848	-6.204	1.00	0.00
ATOM	2296	N	GLU A 662	-17.646	15.274	-6.688	1.00	0.00
ATOM	2297	CA	GLU A 662	-16.412	15.526	-7.380	1.00	0.00
ATOM	2298	C	GLU A 662	-15.564	14.293	-7.315	1.00	0.00
ATOM	2299	O	GLU A 662	-15.021	13.830	-8.319	1.00	0.00
ATOM	2300	CB	GLU A 662	-15.568	16.594	-6.662	1.00	0.00
ATOM	2301	CG	GLU A 662	-16.170	17.997	-6.642	1.00	0.00
ATOM	2302	CD	GLU A 662	-15.293	18.914	-7.473	1.00	0.00



63/208

ATOM	2303	OE1	GLU	A	662	-14.265	18.432	-8.015	1.00	0.00
ATOM	2304	OE2	GLU	A	662	-15.631	20.123	-7.555	1.00	0.00
ATOM	2305	HN	GLU	A	662	-17.854	15.812	-5.871	1.00	0.00
ATOM	2306	HA	GLU	A	662	-16.672	15.859	-8.385	1.00	0.00
ATOM	2307	IHB	GLU	A	662	-14.597	16.646	-7.151	1.00	0.00
ATOM	2308	2HB	GLU	A	662	-15.418	16.273	-5.633	1.00	0.00
ATOM	2309	IHG	GLU	A	662	-16.217	18.376	-5.621	1.00	0.00
ATOM	2310	2HG	GLU	A	662	-17.175	17.985	-7.064	1.00	0.00
ATOM	2311	N	TYR	A	663	-15.466	13.711	-6.105	1.00	0.00
ATOM	2312	CA	TYR	A	663	-14.615	12.585	-5.853	1.00	0.00
ATOM	2313	C	TYR	A	663	-14.948	11.458	-6.774	1.00	0.00
ATOM	2314	O	TYR	A	663	-14.074	10.896	-7.433	1.00	0.00
ATOM	2315	CB	TYR	A	663	-14.789	12.093	-4.404	1.00	0.00
ATOM	2316	CG	TYR	A	663	-14.191	10.738	-4.252	1.00	0.00
ATOM	2317	CD1	TYR	A	663	-12.830	10.563	-4.239	1.00	0.00
ATOM	2318	CD2	TYR	A	663	-15.000	9.658	-3.983	1.00	0.00
ATOM	2319	CE1	TYR	A	663	-12.281	9.319	-4.041	1.00	0.00
ATOM	2320	CE2	TYR	A	663	-14.459	8.414	-3.759	1.00	0.00
ATOM	2321	CZ	TYR	A	663	-13.098	8.241	-3.803	1.00	0.00
ATOM	2322	OH	TYR	A	663	-12.537	6.964	-3.581	1.00	0.00
ATOM	2323	HN	TYR	A	663	-16.010	14.080	-5.352	1.00	0.00
ATOM	2324	HA	TYR	A	663	-13.589	12.909	-6.029	1.00	0.00
ATOM	2325	IHB	TYR	A	663	-15.849	12.044	-4.152	1.00	0.00
ATOM	2326	2HB	TYR	A	663	-14.295	12.779	-3.716	1.00	0.00
ATOM	2327	HD1	TYR	A	663	-12.182	11.414	-4.386	1.00	0.00
ATOM	2328	HE1	TYR	A	663	-11.209	9.189	-4.073	1.00	0.00
ATOM	2329	HD2	TYR	A	663	-16.071	9.788	-3.947	1.00	0.00
ATOM	2330	HE2	TYR	A	663	-15.105	7.574	-3.550	1.00	0.00
ATOM	2331	HH	TYR	A	663	-12.965	6.330	-4.140	1.00	0.00
ATOM	2332	N	LEU	A	664	-16.242	11.130	-6.887	1.00	0.00
ATOM	2333	CA	LEU	A	664	-16.646	10.024	-7.700	1.00	0.00
ATOM	2334	C	LEU	A	664	-16.277	10.231	-9.134	1.00	0.00
ATOM	2335	O	LEU	A	664	-15.938	9.278	-9.834	1.00	0.00
ATOM	2336	CB	LEU	A	664	-18.150	9.737	-7.595	1.00	0.00
ATOM	2337	CG	LEU	A	664	-18.516	9.035	-6.274	1.00	0.00
ATOM	2338	CD1	LEU	A	664	-18.042	7.572	-6.264	1.00	0.00
ATOM	2339	CD2	LEU	A	664	-17.958	9.802	-5.070	1.00	0.00
ATOM	2340	HN	LEU	A	664	-16.932	11.663	-6.397	1.00	0.00
ATOM	2341	HA	LEU	A	664	-16.074	9.160	-7.363	1.00	0.00
ATOM	2342	IHB	LEU	A	664	-18.452	9.105	-8.430	1.00	0.00
ATOM	2343	2HB	LEU	A	664	-18.697	10.677	-7.662	1.00	0.00
ATOM	2344	HG	LEU	A	664	-19.597	9.063	-6.140	1.00	0.00
ATOM	2345	IHD1	LEU	A	664	-17.391	7.372	-7.115	1.00	0.00
ATOM	2346	2HD1	LEU	A	664	-18.897	6.899	-6.329	1.00	0.00
ATOM	2347	3HD1	LEU	A	664	-17.481	7.364	-5.353	1.00	0.00
ATOM	2348	IHD2	LEU	A	664	-18.594	10.652	-4.826	1.00	0.00
ATOM	2349	2HD2	LEU	A	664	-16.961	10.181	-5.295	1.00	0.00
ATOM	2350	3HD2	LEU	A	664	-17.914	9.152	-4.196	1.00	0.00
ATOM	2351	N	CYS	A	665	-16.360	11.477	-9.628	1.00	0.00

64/208

ATOM	2352	CA	CYS A 665	-16.026	11.718	-11.002	1.00	0.00
ATOM	2353	C	CYS A 665	-14.559	11.530	-11.271	1.00	0.00
ATOM	2354	O	CYS A 665	-14.176	10.917	-12.267	1.00	0.00
ATOM	2355	CB	CYS A 665	-16.440	13.121	-11.457	1.00	0.00
ATOM	2356	SG	CYS A 665	-18.245	13.318	-11.386	1.00	0.00
ATOM	2357	HN	CYS A 665	-16.652	12.231	-9.041	1.00	0.00
ATOM	2358	HA	CYS A 665	-16.545	10.961	-11.590	1.00	0.00
ATOM	2359	1HB	CYS A 665	-16.109	13.289	-12.482	1.00	0.00
ATOM	2360	2HB	CYS A 665	-15.979	13.869	-10.812	1.00	0.00
ATOM	2361	HG	CYS A 665	-18.563	14.157	-10.398	1.00	0.00
ATOM	2362	N	MET A 666	-13.682	12.032	-10.379	1.00	0.00
ATOM	2363	CA	MET A 666	-12.269	11.910	-10.626	1.00	0.00
ATOM	2364	C	MET A 666	-11.910	10.462	-10.680	1.00	0.00
ATOM	2365	O	MET A 666	-11.143	10.027	-11.537	1.00	0.00
ATOM	2366	CB	MET A 666	-11.385	12.529	-9.528	1.00	0.00
ATOM	2367	CG	MET A 666	-9.890	12.371	-9.834	1.00	0.00
ATOM	2368	SD	MET A 666	-8.751	12.899	-8.518	1.00	0.00
ATOM	2369	CE	MET A 666	-8.679	14.648	-8.996	1.00	0.00
ATOM	2370	HN	MET A 666	-14.012	12.485	-9.551	1.00	0.00
ATOM	2371	HA	MET A 666	-12.080	12.407	-11.577	1.00	0.00
ATOM	2372	1HB	MET A 666	-11.607	12.046	-8.577	1.00	0.00
ATOM	2373	2HB	MET A 666	-11.620	13.589	-9.437	1.00	0.00
ATOM	2374	1HG	MET A 666	-9.656	12.955	-10.723	1.00	0.00
ATOM	2375	2HG	MET A 666	-9.689	11.320	-10.038	1.00	0.00
ATOM	2376	1HE	MET A 666	-9.197	15.250	-8.250	1.00	0.00
ATOM	2377	2HE	MET A 666	-9.169	14.789	-9.959	1.00	0.00
ATOM	2378	3HE	MET A 666	-7.641	14.975	-9.048	1.00	0.00
ATOM	2379	N	LYS A 667	-12.496	9.665	-9.774	1.00	0.00
ATOM	2380	CA	LYS A 667	-12.171	8.276	-9.706	1.00	0.00
ATOM	2381	C	LYS A 667	-12.427	7.639	-11.042	1.00	0.00
ATOM	2382	O	LYS A 667	-11.599	6.877	-11.541	1.00	0.00
ATOM	2383	CB	LYS A 667	-13.029	7.561	-8.645	1.00	0.00
ATOM	2384	CG	LYS A 667	-12.738	6.070	-8.521	1.00	0.00
ATOM	2385	CD	LYS A 667	-13.243	5.424	-7.228	1.00	0.00
ATOM	2386	CE	LYS A 667	-14.595	5.945	-6.740	1.00	0.00
ATOM	2387	NZ	LYS A 667	-15.045	5.151	-5.575	1.00	0.00
ATOM	2388	HN	LYS A 667	-13.166	10.049	-9.139	1.00	0.00
ATOM	2389	HA	LYS A 667	-11.113	8.205	-9.454	1.00	0.00
ATOM	2390	1HB	LYS A 667	-14.079	7.690	-8.903	1.00	0.00
ATOM	2391	2HB	LYS A 667	-12.852	8.032	-7.680	1.00	0.00
ATOM	2392	1HG	LYS A 667	-11.660	5.925	-8.579	1.00	0.00
ATOM	2393	2HG	LYS A 667	-13.200	5.559	-9.364	1.00	0.00
ATOM	2394	1HD	LYS A 667	-12.505	5.596	-6.446	1.00	0.00
ATOM	2395	2HD	LYS A 667	-13.326	4.350	-7.390	1.00	0.00
ATOM	2396	1HE	LYS A 667	-15.345	5.853	-7.526	1.00	0.00
ATOM	2397	2HE	LYS A 667	-14.513	6.987	-6.432	1.00	0.00
ATOM	2398	1HZ	LYS A 667	-14.346	5.234	-4.809	1.00	0.00
ATOM	2399	2HZ	LYS A 667	-15.139	4.153	-5.851	1.00	0.00
ATOM	2400	3HZ	LYS A 667	-15.964	5.508	-5.246	1.00	0.00

65/208

ATOM 2401 N THR A 668	-13.575	7.951	-11.671	1.00	0.00
ATOM 2402 CA THR A 668	-13.899	7.362	-12.940	1.00	0.00
ATOM 2403 C THR A 668	-12.923	7.822	-13.968	1.00	0.00
ATOM 2404 O THR A 668	-12.511	7.056	-14.838	1.00	0.00
ATOM 2405 CB THR A 668	-15.262	7.745	-13.429	1.00	0.00
ATOM 2406 OG1 THR A 668	-15.314	9.130	-13.734	1.00	0.00
ATOM 2407 CG2 THR A 668	-16.267	7.419	-12.316	1.00	0.00
ATOM 2408 HN THR A 668	-14.208	8.600	-11.250	1.00	0.00
ATOM 2409 HA THR A 668	-13.840	6.282	-12.807	1.00	0.00
ATOM 2410 HB THR A 668	-15.506	7.190	-14.335	1.00	0.00
ATOM 2411 HG1 THR A 668	-14.822	9.577	-13.058	1.00	0.00
ATOM 2412 IHG2 THR A 668	-16.142	8.099	-11.473	1.00	0.00
ATOM 2413 2HG2 THR A 668	-16.112	6.403	-11.955	1.00	0.00
ATOM 2414 3HG2 THR A 668	-17.286	7.526	-12.686	1.00	0.00
ATOM 2415 N LEU A 669	-12.528	9.103	-13.882	1.00	0.00
ATOM 2416 CA LEU A 669	-11.627	9.672	-14.836	1.00	0.00
ATOM 2417 C LEU A 669	-10.377	8.854	-14.779	1.00	0.00
ATOM 2418 O LEU A 669	-9.848	8.427	-15.801	1.00	0.00
ATOM 2419 CB LEU A 669	-11.252	11.117	-14.451	1.00	0.00
ATOM 2420 CG LEU A 669	-10.406	11.869	-15.492	1.00	0.00
ATOM 2421 CD1 LEU A 669	-11.238	12.181	-16.744	1.00	0.00
ATOM 2422 CD2 LEU A 669	-9.759	13.126	-14.890	1.00	0.00
ATOM 2423 HN LEU A 669	-12.873	9.671	-13.134	1.00	0.00
ATOM 2424 HA LEU A 669	-12.129	9.653	-15.803	1.00	0.00
ATOM 2425 IHB LEU A 669	-10.697	11.089	-13.514	1.00	0.00
ATOM 2426 2HB LEU A 669	-12.172	11.677	-14.288	1.00	0.00
ATOM 2427 HG LEU A 669	-9.547	11.259	-15.769	1.00	0.00
ATOM 2428 IHD1 LEU A 669	-12.097	12.801	-16.491	1.00	0.00
ATOM 2429 2HD1 LEU A 669	-11.609	11.258	-17.189	1.00	0.00
ATOM 2430 3HD1 LEU A 669	-10.634	12.722	-17.472	1.00	0.00
ATOM 2431 IHD2 LEU A 669	-9.564	12.988	-13.827	1.00	0.00
ATOM 2432 2HD2 LEU A 669	-10.424	13.982	-15.003	1.00	0.00
ATOM 2433 3HD2 LEU A 669	-8.809	13.333	-15.383	1.00	0.00
ATOM 2434 N LEU A 670	-9.878	8.557	-13.571	1.00	0.00
ATOM 2435 CA LEU A 670	-8.653	7.820	-13.524	1.00	0.00
ATOM 2436 C LEU A 670	-8.775	6.453	-14.115	1.00	0.00
ATOM 2437 O LEU A 670	-7.844	5.969	-14.757	1.00	0.00
ATOM 2438 CB LEU A 670	-8.036	7.728	-12.123	1.00	0.00
ATOM 2439 CG LEU A 670	-7.389	9.061	-11.706	1.00	0.00
ATOM 2440 CD1 LEU A 670	-6.275	9.444	-12.693	1.00	0.00
ATOM 2441 CD2 LEU A 670	-8.411	10.188	-11.504	1.00	0.00
ATOM 2442 HN LEU A 670	-10.346	8.841	-12.735	1.00	0.00
ATOM 2443 HA LEU A 670	-7.963	8.326	-14.199	1.00	0.00
ATOM 2444 IHB LEU A 670	-7.280	6.943	-12.114	1.00	0.00
ATOM 2445 2HB LEU A 670	-8.812	7.464	-11.405	1.00	0.00
ATOM 2446 HG LEU A 670	-6.972	8.967	-10.703	1.00	0.00
ATOM 2447 IHD1 LEU A 670	-6.696	9.727	-13.658	1.00	0.00
ATOM 2448 2HD1 LEU A 670	-5.606	8.599	-12.852	1.00	0.00
ATOM 2449 3HD1 LEU A 670	-5.709	10.293	-12.311	1.00	0.00

66/208

ATOM	2450	1HD2 LEU A 670	-9.306	9.812	-11.010	1.00	0.00
ATOM	2451	2HD2 LEU A 670	-8.707	10.604	-12.467	1.00	0.00
ATOM	2452	3HD2 LEU A 670	-7.986	10.974	-10.880	1.00	0.00
ATOM	2453	N LEU A 671	-9.926	5.787	-13.931	1.00	0.00
ATOM	2454	CA LEU A 671	-10.044	4.459	-14.453	1.00	0.00
ATOM	2455	C LEU A 671	-9.944	4.433	-15.955	1.00	0.00
ATOM	2456	O LEU A 671	-9.366	3.509	-16.522	1.00	0.00
ATOM	2457	CB LEU A 671	-11.309	3.731	-13.950	1.00	0.00
ATOM	2458	CG LEU A 671	-11.475	2.292	-14.479	1.00	0.00
ATOM	2459	CD1 LEU A 671	-12.424	1.474	-13.594	1.00	0.00
ATOM	2460	CD2 LEU A 671	-11.975	2.298	-15.931	1.00	0.00
ATOM	2461	HN LEU A 671	-10.685	6.211	-13.438	1.00	0.00
ATOM	2462	HA LEU A 671	-9.151	3.919	-14.139	1.00	0.00
ATOM	2463	1HB LEU A 671	-12.181	4.311	-14.250	1.00	0.00
ATOM	2464	2HB LEU A 671	-11.277	3.697	-12.862	1.00	0.00
ATOM	2465	HG LEU A 671	-10.501	1.805	-14.507	1.00	0.00
ATOM	2466	1HD1 LEU A 671	-13.450	1.827	-13.700	1.00	0.00
ATOM	2467	2HD1 LEU A 671	-12.140	1.571	-12.547	1.00	0.00
ATOM	2468	3HD1 LEU A 671	-12.398	0.424	-13.885	1.00	0.00
ATOM	2469	1HD2 LEU A 671	-12.110	3.319	-16.288	1.00	0.00
ATOM	2470	2HD2 LEU A 671	-12.936	1.787	-16.000	1.00	0.00
ATOM	2471	3HD2 LEU A 671	-11.251	1.806	-16.580	1.00	0.00
ATOM	2472	N LEU A 672	-10.499	5.448	-16.647	1.00	0.00
ATOM	2473	CA LEU A 672	-10.544	5.514	-18.089	1.00	0.00
ATOM	2474	C LEU A 672	-9.324	5.736	-18.977	1.00	0.00
ATOM	2475	O LEU A 672	-9.312	5.224	-20.093	1.00	0.00
ATOM	2476	CB LEU A 672	-11.620	6.488	-18.600	1.00	0.00
ATOM	2477	CG LEU A 672	-13.033	5.882	-18.591	1.00	0.00
ATOM	2478	CD1 LEU A 672	-13.210	4.877	-19.740	1.00	0.00
ATOM	2479	CD2 LEU A 672	-13.351	5.236	-17.239	1.00	0.00
ATOM	2480	HN LEU A 672	-10.904	6.201	-16.129	1.00	0.00
ATOM	2481	HA LEU A 672	-10.751	4.505	-18.444	1.00	0.00
ATOM	2482	1HB LEU A 672	-11.371	6.786	-19.618	1.00	0.00
ATOM	2483	2HB LEU A 672	-11.615	7.379	-17.972	1.00	0.00
ATOM	2484	HG LEU A 672	-13.769	6.679	-18.692	1.00	0.00
ATOM	2485	1HD1 LEU A 672	-12.388	4.161	-19.756	1.00	0.00
ATOM	2486	2HD1 LEU A 672	-13.222	5.398	-20.697	1.00	0.00
ATOM	2487	3HD1 LEU A 672	-14.139	4.321	-19.614	1.00	0.00
ATOM	2488	1HD2 LEU A 672	-12.588	5.489	-16.503	1.00	0.00
ATOM	2489	2HD2 LEU A 672	-13.379	4.151	-17.337	1.00	0.00
ATOM	2490	3HD2 LEU A 672	-14.310	5.596	-16.867	1.00	0.00
ATOM	2491	N SER A 673	-8.272	6.488	-18.577	1.00	0.00
ATOM	2492	CA SER A 673	-7.270	6.880	-19.559	1.00	0.00
ATOM	2493	C SER A 673	-6.215	5.842	-19.924	1.00	0.00
ATOM	2494	O SER A 673	-5.320	5.609	-19.119	1.00	0.00
ATOM	2495	CB SER A 673	-6.473	8.135	-19.153	1.00	0.00
ATOM	2496	OG SER A 673	-7.309	9.282	-19.137	1.00	0.00
ATOM	2497	HN SER A 673	-8.185	6.770	-17.621	1.00	0.00
ATOM	2498	HA SER A 673	-7.805	7.063	-20.491	1.00	0.00

67/208

ATOM	2499	IHB	SER A 673	-5.667	8.315	-19.866	1.00	0.00
ATOM	2500	2HB	SER A 673	-6.055	8.007	-18.155	1.00	0.00
ATOM	2501	HG	SER A 673	-8.075	9.053	-18.627	1.00	0.00
ATOM	2502	N	SER A 674	-6.229	5.234	-21.156	1.00	0.00
ATOM	2503	CA	SER A 674	-5.225	4.221	-21.490	1.00	0.00
ATOM	2504	C	SER A 674	-5.519	3.470	-22.793	1.00	0.00
ATOM	2505	O	SER A 674	-6.620	3.564	-23.322	1.00	0.00
ATOM	2506	CB	SER A 674	-5.151	3.147	-20.380	1.00	0.00
ATOM	2507	OG	SER A 674	-4.245	2.107	-20.714	1.00	0.00
ATOM	2508	HN	SER A 674	-6.927	5.485	-21.827	1.00	0.00
ATOM	2509	HA	SER A 674	-4.270	4.734	-21.594	1.00	0.00
ATOM	2510	IHB	SER A 674	-6.133	2.699	-20.231	1.00	0.00
ATOM	2511	2HB	SER A 674	-4.811	3.599	-19.448	1.00	0.00
ATOM	2512	HG	SER A 674	-4.370	1.421	-20.072	1.00	0.00
ATOM	2513	N	VAL A 675	-4.521	2.672	-23.293	1.00	0.00
ATOM	2514	CA	VAL A 675	-4.423	1.847	-24.498	1.00	0.00
ATOM	2515	C	VAL A 675	-5.492	0.778	-24.497	1.00	0.00
ATOM	2516	O	VAL A 675	-6.542	1.113	-23.963	1.00	0.00
ATOM	2517	CB	VAL A 675	-3.003	1.312	-24.570	1.00	0.00
ATOM	2518	CG1	VAL A 675	-2.839	0.093	-23.643	1.00	0.00
ATOM	2519	CG2	VAL A 675	-2.509	1.219	-26.026	1.00	0.00
ATOM	2520	HN	VAL A 675	-3.705	2.649	-22.725	1.00	0.00
ATOM	2521	HA	VAL A 675	-4.654	2.476	-25.357	1.00	0.00
ATOM	2522	HB	VAL A 675	-2.304	2.093	-24.273	1.00	0.00
ATOM	2523	IHG1	VAL A 675	-3.780	-0.449	-23.550	1.00	0.00
ATOM	2524	2HG1	VAL A 675	-2.536	0.416	-22.647	1.00	0.00
ATOM	2525	3HG1	VAL A 675	-2.095	-0.591	-24.049	1.00	0.00
ATOM	2526	IHG2	VAL A 675	-1.874	2.069	-26.273	1.00	0.00
ATOM	2527	2HG2	VAL A 675	-3.357	1.221	-26.712	1.00	0.00
ATOM	2528	3HG2	VAL A 675	-1.925	0.310	-26.168	1.00	0.00
ATOM	2529	N	PRO A 676	-5.477	-0.434	-25.043	1.00	0.00
ATOM	2530	CA	PRO A 676	-4.453	-1.012	-25.884	1.00	0.00
ATOM	2531	C	PRO A 676	-4.796	-0.749	-27.315	1.00	0.00
ATOM	2532	O	PRO A 676	-5.914	-0.312	-27.586	1.00	0.00
ATOM	2533	CB	PRO A 676	-4.440	-2.512	-25.580	1.00	0.00
ATOM	2534	CG	PRO A 676	-5.840	-2.792	-25.019	1.00	0.00
ATOM	2535	CD	PRO A 676	-6.217	-1.471	-24.338	1.00	0.00
ATOM	2536	IHD	PRO A 676	-7.288	-1.284	-24.415	1.00	0.00
ATOM	2537	2HD	PRO A 676	-5.937	-1.481	-23.285	1.00	0.00
ATOM	2538	HA	PRO A 676	-3.487	-0.562	-25.656	1.00	0.00
ATOM	2539	IHB	PRO A 676	-3.668	-2.759	-24.852	1.00	0.00
ATOM	2540	2HB	PRO A 676	-4.255	-3.094	-26.483	1.00	0.00
ATOM	2541	IHG	PRO A 676	-6.543	-3.044	-25.813	1.00	0.00
ATOM	2542	2HG	PRO A 676	-5.823	-3.615	-24.304	1.00	0.00
ATOM	2543	N	LYS A 677	-3.859	-1.003	-28.252	1.00	0.00
ATOM	2544	CA	LYS A 677	-4.201	-0.796	-29.627	1.00	0.00
ATOM	2545	C	LYS A 677	-4.195	-2.100	-30.367	1.00	0.00
ATOM	2546	O	LYS A 677	-3.171	-2.541	-30.886	1.00	0.00
ATOM	2547	CB	LYS A 677	-3.275	0.192	-30.374	1.00	0.00

68/208

ATOM	2548	CG	LYS A 677	-1.800	-0.215	-30.473	1.00	0.00
ATOM	2549	CD	LYS A 677	-1.037	0.541	-31.565	1.00	0.00
ATOM	2550	CE	LYS A 677	0.377	0.011	-31.813	1.00	0.00
ATOM	2551	NZ	LYS A 677	0.959	0.660	-33.010	1.00	0.00
ATOM	2552	HN	LYS A 677	-2.949	-1.328	-27.992	1.00	0.00
ATOM	2553	HA	LYS A 677	-5.223	-0.419	-29.633	1.00	0.00
ATOM	2554	1HB	LYS A 677	-3.327	1.153	-29.866	1.00	0.00
ATOM	2555	2HB	LYS A 677	-3.659	0.316	-31.385	1.00	0.00
ATOM	2556	1HG	LYS A 677	-1.743	-1.283	-30.680	1.00	0.00
ATOM	2557	2HG	LYS A 677	-1.319	-0.026	-29.514	1.00	0.00
ATOM	2558	1HD	LYS A 677	-0.970	1.590	-31.280	1.00	0.00
ATOM	2559	2HD	LYS A 677	-1.601	0.474	-32.494	1.00	0.00
ATOM	2560	1HE	LYS A 677	0.354	-1.065	-31.986	1.00	0.00
ATOM	2561	2HE	LYS A 677	1.020	0.231	-30.961	1.00	0.00
ATOM	2562	1HZ	LYS A 677	1.000	1.688	-32.862	1.00	0.00
ATOM	2563	2HZ	LYS A 677	0.366	0.453	-33.839	1.00	0.00
ATOM	2564	3HZ	LYS A 677	1.919	0.294	-33.171	1.00	0.00
ATOM	2565	N	ASP A 678	-5.355	-2.780	-30.419	1.00	0.00
ATOM	2566	CA	ASP A 678	-5.403	-3.975	-31.206	1.00	0.00
ATOM	2567	C	ASP A 678	-5.302	-3.500	-32.613	1.00	0.00
ATOM	2568	O	ASP A 678	-4.614	-4.095	-33.442	1.00	0.00
ATOM	2569	CB	ASP A 678	-6.712	-4.768	-31.063	1.00	0.00
ATOM	2570	CG	ASP A 678	-6.667	-5.508	-29.735	1.00	0.00
ATOM	2571	OD1	ASP A 678	-7.705	-6.119	-29.363	1.00	0.00
ATOM	2572	OD2	ASP A 678	-5.594	-5.476	-29.076	1.00	0.00
ATOM	2573	HN	ASP A 678	-6.161	-2.459	-29.921	1.00	0.00
ATOM	2574	HA	ASP A 678	-4.562	-4.588	-30.882	1.00	0.00
ATOM	2575	1HB	ASP A 678	-6.815	-5.488	-31.875	1.00	0.00
ATOM	2576	2HB	ASP A 678	-7.571	-4.096	-31.073	1.00	0.00
ATOM	2577	N	GLY A 679	-5.989	-2.381	-32.908	1.00	0.00
ATOM	2578	CA	GLY A 679	-5.943	-1.827	-34.223	1.00	0.00
ATOM	2579	C	GLY A 679	-7.129	-0.938	-34.393	1.00	0.00
ATOM	2580	O	GLY A 679	-7.322	0.016	-33.642	1.00	0.00
ATOM	2581	HN	GLY A 679	-6.535	-1.934	-32.199	1.00	0.00
ATOM	2582	1HA	GLY A 679	-5.978	-2.646	-34.940	1.00	0.00
ATOM	2583	2HA	GLY A 679	-5.023	-1.253	-34.321	1.00	0.00
ATOM	2584	N	LEU A 680	-7.974	-1.247	-35.390	1.00	0.00
ATOM	2585	CA	LEU A 680	-9.110	-0.416	-35.644	1.00	0.00
ATOM	2586	C	LEU A 680	-9.988	-0.447	-34.444	1.00	0.00
ATOM	2587	O	LEU A 680	-10.549	0.573	-34.047	1.00	0.00
ATOM	2588	CB	LEU A 680	-9.935	-0.874	-36.858	1.00	0.00
ATOM	2589	CG	LEU A 680	-9.171	-0.731	-38.187	1.00	0.00
ATOM	2590	CD1	LEU A 680	-7.937	-1.648	-38.224	1.00	0.00
ATOM	2591	CD2	LEU A 680	-10.102	-0.926	-39.392	1.00	0.00
ATOM	2592	HN	LEU A 680	-7.809	-2.056	-35.954	1.00	0.00
ATOM	2593	HA	LEU A 680	-8.728	0.591	-35.810	1.00	0.00
ATOM	2594	1HB	LEU A 680	-10.847	-0.280	-36.909	1.00	0.00
ATOM	2595	2HB	LEU A 680	-10.214	-1.918	-36.722	1.00	0.00
ATOM	2596	HG	LEU A 680	-8.853	0.304	-38.310	1.00	0.00

ATOM	2597	1HD1	LEU	A	680	-8.164	-2.616	-37.778	1.00	0.00
ATOM	2598	2HD1	LEU	A	680	-7.118	-1.201	-37.661	1.00	0.00
ATOM	2599	3HD1	LEU	A	680	-7.625	-1.816	-39.255	1.00	0.00
ATOM	2600	1HD2	LEU	A	680	-10.902	-0.186	-39.385	1.00	0.00
ATOM	2601	2HD2	LEU	A	680	-10.558	-1.916	-39.359	1.00	0.00
ATOM	2602	3HD2	LEU	A	680	-9.544	-0.811	-40.321	1.00	0.00
ATOM	2603	N	LYS	A	681	-10.116	-1.628	-33.820	1.00	0.00
ATOM	2604	CA	LYS	A	681	-10.950	-1.737	-32.666	1.00	0.00
ATOM	2605	C	LYS	A	681	-10.397	-0.839	-31.612	1.00	0.00
ATOM	2606	O	LYS	A	681	-11.152	-0.186	-30.892	1.00	0.00
ATOM	2607	CB	LYS	A	681	-10.994	-3.159	-32.086	1.00	0.00
ATOM	2608	CG	LYS	A	681	-11.782	-4.143	-32.953	1.00	0.00
ATOM	2609	CD	LYS	A	681	-13.264	-3.791	-33.083	1.00	0.00
ATOM	2610	CE	LYS	A	681	-14.052	-4.774	-33.949	1.00	0.00
ATOM	2611	NZ	LYS	A	681	-13.595	-4.689	-35.355	1.00	0.00
ATOM	2612	HN	LYS	A	681	-9.628	-2.430	-34.164	1.00	0.00
ATOM	2613	HA	LYS	A	681	-11.949	-1.428	-32.973	1.00	0.00
ATOM	2614	1HB	LYS	A	681	-11.449	-3.121	-31.097	1.00	0.00
ATOM	2615	2HB	LYS	A	681	-9.974	-3.526	-31.979	1.00	0.00
ATOM	2616	1HG	LYS	A	681	-11.696	-5.138	-32.518	1.00	0.00
ATOM	2617	2HG	LYS	A	681	-11.339	-4.164	-33.947	1.00	0.00
ATOM	2618	1HD	LYS	A	681	-13.349	-2.796	-33.519	1.00	0.00
ATOM	2619	2HD	LYS	A	681	-13.707	-3.768	-32.089	1.00	0.00
ATOM	2620	1HE	LYS	A	681	-15.115	-4.536	-33.922	1.00	0.00
ATOM	2621	2HE	LYS	A	681	-13.897	-5.795	-33.601	1.00	0.00
ATOM	2622	1HZ	LYS	A	681	-12.583	-4.924	-35.405	1.00	0.00
ATOM	2623	2HZ	LYS	A	681	-13.744	-3.724	-35.711	1.00	0.00
ATOM	2624	3HZ	LYS	A	681	-14.135	-5.361	-35.937	1.00	0.00
ATOM	2625	N	SER	A	682	-9.058	-0.771	-31.496	1.00	0.00
ATOM	2626	CA	SER	A	682	-8.516	0.051	-30.459	1.00	0.00
ATOM	2627	C	SER	A	682	-8.919	1.467	-30.694	1.00	0.00
ATOM	2628	O	SER	A	682	-9.388	2.127	-29.772	1.00	0.00
ATOM	2629	CB	SER	A	682	-6.978	0.012	-30.339	1.00	0.00
ATOM	2630	OG	SER	A	682	-6.366	0.766	-31.373	1.00	0.00
ATOM	2631	HN	SER	A	682	-8.462	-1.280	-32.115	1.00	0.00
ATOM	2632	HA	SER	A	682	-8.965	-0.299	-29.529	1.00	0.00
ATOM	2633	1HB	SER	A	682	-6.623	-1.016	-30.417	1.00	0.00
ATOM	2634	2HB	SER	A	682	-6.667	0.434	-29.384	1.00	0.00
ATOM	2635	HG	SER	A	682	-7.010	0.857	-32.062	1.00	0.00
ATOM	2636	N	GLN	A	683	-8.804	1.975	-31.937	1.00	0.00
ATOM	2637	CA	GLN	A	683	-9.159	3.355	-32.108	1.00	0.00
ATOM	2638	C	GLN	A	683	-10.607	3.525	-31.795	1.00	0.00
ATOM	2639	O	GLN	A	683	-11.012	4.550	-31.250	1.00	0.00
ATOM	2640	CB	GLN	A	683	-8.907	3.961	-33.504	1.00	0.00
ATOM	2641	CG	GLN	A	683	-9.702	3.344	-34.655	1.00	0.00
ATOM	2642	CD	GLN	A	683	-8.737	2.506	-35.476	1.00	0.00
ATOM	2643	OE1	GLN	A	683	-7.665	2.128	-35.005	1.00	0.00
ATOM	2644	NE2	GLN	A	683	-9.115	2.226	-36.752	1.00	0.00
ATOM	2645	HN	GLN	A	683	-8.486	1.417	-32.703	1.00	0.00

70/208

ATOM	2646	HA	GLN A 683	-8.576	3.903	-31.368	1.00	0.00
ATOM	2647	1HB	GLN A 683	-7.848	3.855	-33.731	1.00	0.00
ATOM	2648	2HB	GLN A 683	-9.146	5.022	-33.459	1.00	0.00
ATOM	2649	1HG	GLN A 683	-10.134	4.122	-35.285	1.00	0.00
ATOM	2650	2HG	GLN A 683	-10.502	2.709	-34.274	1.00	0.00
ATOM	2651	1HE2	GLN A 683	-8.460	1.811	-37.383	1.00	0.00
ATOM	2652	2HE2	GLN A 683	-10.039	2.429	-37.075	1.00	0.00
ATOM	2653	N	GLU A 684	-11.433	2.521	-32.140	1.00	0.00
ATOM	2654	CA	GLU A 684	-12.839	2.607	-31.877	1.00	0.00
ATOM	2655	C	GLU A 684	-13.018	2.688	-30.394	1.00	0.00
ATOM	2656	O	GLU A 684	-13.812	3.478	-29.888	1.00	0.00
ATOM	2657	CB	GLU A 684	-13.597	1.362	-32.363	1.00	0.00
ATOM	2658	CG	GLU A 684	-15.098	1.590	-32.521	1.00	0.00
ATOM	2659	CD	GLU A 684	-15.285	2.313	-33.845	1.00	0.00
ATOM	2660	OE1	GLU A 684	-14.495	2.028	-34.784	1.00	0.00
ATOM	2661	OE2	GLU A 684	-16.211	3.162	-33.936	1.00	0.00
ATOM	2662	HN	GLU A 684	-11.061	1.706	-32.584	1.00	0.00
ATOM	2663	HA	GLU A 684	-13.203	3.496	-32.392	1.00	0.00
ATOM	2664	1HB	GLU A 684	-13.438	0.554	-31.649	1.00	0.00
ATOM	2665	2HB	GLU A 684	-13.186	1.055	-33.324	1.00	0.00
ATOM	2666	1HG	GLU A 684	-15.486	2.204	-31.708	1.00	0.00
ATOM	2667	2HG	GLU A 684	-15.636	0.642	-32.540	1.00	0.00
ATOM	2668	N	LEU A 685	-12.256	1.860	-29.660	1.00	0.00
ATOM	2669	CA	LEU A 685	-12.333	1.834	-28.230	1.00	0.00
ATOM	2670	C	LEU A 685	-11.900	3.180	-27.745	1.00	0.00
ATOM	2671	O	LEU A 685	-12.485	3.719	-26.809	1.00	0.00
ATOM	2672	CB	LEU A 685	-11.418	0.741	-27.624	1.00	0.00
ATOM	2673	CG	LEU A 685	-11.464	0.523	-26.089	1.00	0.00
ATOM	2674	CD1	LEU A 685	-10.495	-0.600	-25.688	1.00	0.00
ATOM	2675	CD2	LEU A 685	-11.179	1.793	-25.269	1.00	0.00
ATOM	2676	HN	LEU A 685	-11.618	1.246	-30.124	1.00	0.00
ATOM	2677	HA	LEU A 685	-13.374	1.643	-27.972	1.00	0.00
ATOM	2678	1HB	LEU A 685	-10.393	0.988	-27.890	1.00	0.00
ATOM	2679	2HB	LEU A 685	-11.679	-0.203	-28.097	1.00	0.00
ATOM	2680	HG	LEU A 685	-12.477	0.258	-25.787	1.00	0.00
ATOM	2681	1HD1	LEU A 685	-9.565	-0.186	-25.300	1.00	0.00
ATOM	2682	2HD1	LEU A 685	-10.254	-1.217	-26.554	1.00	0.00
ATOM	2683	3HD1	LEU A 685	-10.939	-1.220	-24.909	1.00	0.00
ATOM	2684	1HD2	LEU A 685	-12.108	2.238	-24.912	1.00	0.00
ATOM	2685	2HD2	LEU A 685	-10.667	2.532	-25.886	1.00	0.00
ATOM	2686	3HD2	LEU A 685	-10.566	1.552	-24.401	1.00	0.00
ATOM	2687	N	PHE A 686	-10.863	3.764	-28.371	1.00	0.00
ATOM	2688	CA	PHE A 686	-10.358	5.027	-27.916	1.00	0.00
ATOM	2689	C	PHE A 686	-11.389	6.090	-28.050	1.00	0.00
ATOM	2690	O	PHE A 686	-11.546	6.926	-27.162	1.00	0.00
ATOM	2691	CB	PHE A 686	-9.101	5.529	-28.657	1.00	0.00
ATOM	2692	CG	PHE A 686	-7.902	4.803	-28.143	1.00	0.00
ATOM	2693	CD1	PHE A 686	-7.383	3.716	-28.806	1.00	0.00
ATOM	2694	CD2	PHE A 686	-7.315	5.198	-26.963	1.00	0.00



71/208

ATOM	2695	CE1 PHE A 686	-6.291	3.042	-28.311	1.00	0.00
ATOM	2696	CE2 PHE A 686	-6.225	4.527	-26.460	1.00	0.00
ATOM	2697	CZ PHE A 686	-5.709	3.448	-27.134	1.00	0.00
ATOM	2698	HN PHE A 686	-10.442	3.314	-29.159	1.00	0.00
ATOM	2699	HA PHE A 686	-10.131	4.898	-26.858	1.00	0.00
ATOM	2700	1HB PHE A 686	-8.971	6.599	-28.491	1.00	0.00
ATOM	2701	2HB PHE A 686	-9.199	5.348	-29.727	1.00	0.00
ATOM	2702	HD1 PHE A 686	-7.839	3.387	-29.728	1.00	0.00
ATOM	2703	HD2 PHE A 686	-7.715	6.044	-26.425	1.00	0.00
ATOM	2704	HE1 PHE A 686	-5.891	2.195	-28.848	1.00	0.00
ATOM	2705	HE2 PHE A 686	-5.773	4.850	-25.534	1.00	0.00
ATOM	2706	HZ PHE A 686	-4.852	2.920	-26.742	1.00	0.00
ATOM	2707	N ASP A 687	-12.135	6.092	-29.164	1.00	0.00
ATOM	2708	CA ASP A 687	-13.083	7.148	-29.329	1.00	0.00
ATOM	2709	C ASP A 687	-14.094	7.068	-28.235	1.00	0.00
ATOM	2710	O ASP A 687	-14.430	8.074	-27.612	1.00	0.00
ATOM	2711	CB ASP A 687	-13.841	7.083	-30.663	1.00	0.00
ATOM	2712	CG ASP A 687	-14.550	8.418	-30.818	1.00	0.00
ATOM	2713	OD1 ASP A 687	-14.445	9.244	-29.873	1.00	0.00
ATOM	2714	OD2 ASP A 687	-15.199	8.632	-31.876	1.00	0.00
ATOM	2715	HN ASP A 687	-12.030	5.378	-29.856	1.00	0.00
ATOM	2716	HA ASP A 687	-12.523	8.080	-29.263	1.00	0.00
ATOM	2717	1HB ASP A 687	-14.573	6.276	-30.656	1.00	0.00
ATOM	2718	2HB ASP A 687	-13.153	6.933	-31.495	1.00	0.00
ATOM	2719	N GLU A 688	-14.578	5.849	-27.942	1.00	0.00
ATOM	2720	CA GLU A 688	-15.609	5.742	-26.962	1.00	0.00
ATOM	2721	C GLU A 688	-15.131	6.282	-25.656	1.00	0.00
ATOM	2722	O GLU A 688	-15.805	7.105	-25.037	1.00	0.00
ATOM	2723	CB GLU A 688	-16.078	4.297	-26.724	1.00	0.00
ATOM	2724	CG GLU A 688	-17.293	4.220	-25.797	1.00	0.00
ATOM	2725	CD GLU A 688	-17.856	2.809	-25.859	1.00	0.00
ATOM	2726	OE1 GLU A 688	-17.087	1.874	-26.206	1.00	0.00
ATOM	2727	OE2 GLU A 688	-19.070	2.652	-25.564	1.00	0.00
ATOM	2728	HN GLU A 688	-14.223	5.035	-28.402	1.00	0.00
ATOM	2729	HA GLU A 688	-16.441	6.349	-27.319	1.00	0.00
ATOM	2730	1HB GLU A 688	-15.260	3.727	-26.283	1.00	0.00
ATOM	2731	2HB GLU A 688	-16.333	3.845	-27.681	1.00	0.00
ATOM	2732	1HG GLU A 688	-18.059	4.926	-26.116	1.00	0.00
ATOM	2733	2HG GLU A 688	-17.004	4.446	-24.771	1.00	0.00
ATOM	2734	N ILE A 689	-13.936	5.865	-25.202	1.00	0.00
ATOM	2735	CA ILE A 689	-13.526	6.370	-23.928	1.00	0.00
ATOM	2736	C ILE A 689	-13.262	7.842	-23.953	1.00	0.00
ATOM	2737	O ILE A 689	-13.552	8.537	-22.983	1.00	0.00
ATOM	2738	CB ILE A 689	-12.444	5.577	-23.235	1.00	0.00
ATOM	2739	CG1 ILE A 689	-11.151	5.446	-24.042	1.00	0.00
ATOM	2740	CG2 ILE A 689	-13.060	4.229	-22.839	1.00	0.00
ATOM	2741	CD1 ILE A 689	-10.067	4.699	-23.265	1.00	0.00
ATOM	2742	HN ILE A 689	-13.365	5.235	-25.728	1.00	0.00
ATOM	2743	HA ILE A 689	-14.422	6.382	-23.309	1.00	0.00

72/208

ATOM	2744	HB	ILE A 689	-12.091	6.109	-22.350	1.00	0.00
ATOM	2745	1HG2	ILE A 689	-13.250	3.618	-23.722	1.00	0.00
ATOM	2746	2HG2	ILE A 689	-14.010	4.384	-22.327	1.00	0.00
ATOM	2747	3HG2	ILE A 689	-12.379	3.679	-22.189	1.00	0.00
ATOM	2748	1HG1	ILE A 689	-10.787	6.441	-24.298	1.00	0.00
ATOM	2749	2HG1	ILE A 689	-11.361	4.911	-24.968	1.00	0.00
ATOM	2750	1HD1	ILE A 689	-10.400	3.693	-23.010	1.00	0.00
ATOM	2751	2HD1	ILE A 689	-9.839	5.223	-22.337	1.00	0.00
ATOM	2752	3HD1	ILE A 689	-9.163	4.612	-23.868	1.00	0.00
ATOM	2753	N	ARG A 690	-12.745	8.378	-25.070	1.00	0.00
ATOM	2754	CA	ARG A 690	-12.504	9.793	-25.120	1.00	0.00
ATOM	2755	C	ARG A 690	-13.821	10.474	-24.910	1.00	0.00
ATOM	2756	O	ARG A 690	-13.918	11.457	-24.178	1.00	0.00
ATOM	2757	CB	ARG A 690	-11.949	10.243	-26.483	1.00	0.00
ATOM	2758	CG	ARG A 690	-10.620	9.572	-26.842	1.00	0.00
ATOM	2759	CD	ARG A 690	-10.025	10.023	-28.178	1.00	0.00
ATOM	2760	NE	ARG A 690	-9.259	11.276	-27.924	1.00	0.00
ATOM	2761	CZ	ARG A 690	-8.030	11.450	-28.490	1.00	0.00
ATOM	2762	NH1	ARG A 690	-7.500	10.477	-29.289	1.00	0.00
ATOM	2763	NH2	ARG A 690	-7.324	12.595	-28.252	1.00	0.00
ATOM	2764	HN	ARG A 690	-12.530	7.799	-25.857	1.00	0.00
ATOM	2765	HA	ARG A 690	-11.789	10.018	-24.328	1.00	0.00
ATOM	2766	1HB	ARG A 690	-11.804	11.323	-26.465	1.00	0.00
ATOM	2767	2HB	ARG A 690	-12.680	10.009	-27.256	1.00	0.00
ATOM	2768	1HG	ARG A 690	-10.776	8.495	-26.879	1.00	0.00
ATOM	2769	2HG	ARG A 690	-9.901	9.788	-26.053	1.00	0.00
ATOM	2770	1HD	ARG A 690	-10.805	10.246	-28.905	1.00	0.00
ATOM	2771	2HD	ARG A 690	-9.335	9.280	-28.576	1.00	0.00
ATOM	2772	HE	ARG A 690	-9.645	11.990	-27.339	1.00	0.00
ATOM	2773	1HH1	ARG A 690	-8.014	9.636	-29.460	1.00	0.00
ATOM	2774	2HH1	ARG A 690	-6.599	10.606	-29.703	1.00	0.00
ATOM	2775	1HH2	ARG A 690	-7.708	13.306	-27.663	1.00	0.00
ATOM	2776	2HH2	ARG A 690	-6.423	12.722	-28.667	1.00	0.00
ATOM	2777	N	MET A 691	-14.880	9.937	-25.544	1.00	0.00
ATOM	2778	CA	MET A 691	-16.196	10.500	-25.455	1.00	0.00
ATOM	2779	C	MET A 691	-16.711	10.474	-24.049	1.00	0.00
ATOM	2780	O	MET A 691	-17.297	11.450	-23.583	1.00	0.00
ATOM	2781	CB	MET A 691	-17.218	9.745	-26.318	1.00	0.00
ATOM	2782	CG	MET A 691	-18.627	10.331	-26.228	1.00	0.00
ATOM	2783	SD	MET A 691	-18.833	11.973	-26.976	1.00	0.00
ATOM	2784	CE	MET A 691	-20.569	12.136	-26.468	1.00	0.00
ATOM	2785	HN	MET A 691	-14.743	9.115	-26.097	1.00	0.00
ATOM	2786	HA	MET A 691	-16.117	11.536	-25.785	1.00	0.00
ATOM	2787	1HB	MET A 691	-17.248	8.705	-25.998	1.00	0.00
ATOM	2788	2HB	MET A 691	-16.891	9.774	-27.357	1.00	0.00
ATOM	2789	1HG	MET A 691	-18.904	10.410	-25.178	1.00	0.00
ATOM	2790	2HG	MET A 691	-19.318	9.652	-26.726	1.00	0.00
ATOM	2791	1HE	MET A 691	-20.636	12.085	-25.381	1.00	0.00
ATOM	2792	2HE	MET A 691	-21.157	11.321	-26.891	1.00	0.00

73/208

ATOM	2793	3HE	MET A 691	-20.963	13.097	-26.797	1.00	0.00
ATOM	2794	N	THR A 692	-16.508	9.357	-23.329	1.00	0.00
ATOM	2795	CA	THR A 692	-16.995	9.258	-21.982	1.00	0.00
ATOM	2796	C	THR A 692	-16.283	10.306	-21.199	1.00	0.00
ATOM	2797	O	THR A 692	-16.863	10.948	-20.323	1.00	0.00
ATOM	2798	CB	THR A 692	-16.680	7.937	-21.344	1.00	0.00
ATOM	2799	OG1	THR A 692	-17.264	6.880	-22.089	1.00	0.00
ATOM	2800	CG2	THR A 692	-17.230	7.943	-19.907	1.00	0.00
ATOM	2801	HN	THR A 692	-16.014	8.588	-23.736	1.00	0.00
ATOM	2802	HA	THR A 692	-18.074	9.404	-22.029	1.00	0.00
ATOM	2803	HB	THR A 692	-15.602	7.779	-21.316	1.00	0.00
ATOM	2804	HG1	THR A 692	-16.785	6.824	-22.905	1.00	0.00
ATOM	2805	1HG2	THR A 692	-18.113	8.578	-19.836	1.00	0.00
ATOM	2806	2HG2	THR A 692	-16.480	8.329	-19.218	1.00	0.00
ATOM	2807	3HG2	THR A 692	-17.516	6.934	-19.610	1.00	0.00
ATOM	2808	N	TYR A 693	-14.990	10.511	-21.517	1.00	0.00
ATOM	2809	CA	TYR A 693	-14.227	11.517	-20.844	1.00	0.00
ATOM	2810	C	TYR A 693	-14.929	12.817	-20.883	1.00	0.00
ATOM	2811	O	TYR A 693	-15.150	13.421	-19.838	1.00	0.00
ATOM	2812	CB	TYR A 693	-12.888	11.823	-21.527	1.00	0.00
ATOM	2813	CG	TYR A 693	-11.895	10.964	-20.883	1.00	0.00
ATOM	2814	CD1	TYR A 693	-11.864	9.613	-21.108	1.00	0.00
ATOM	2815	CD2	TYR A 693	-11.090	11.555	-19.944	1.00	0.00
ATOM	2816	CE1	TYR A 693	-11.078	8.830	-20.307	1.00	0.00
ATOM	2817	CE2	TYR A 693	-10.292	10.784	-19.157	1.00	0.00
ATOM	2818	CZ	TYR A 693	-10.331	9.429	-19.322	1.00	0.00
ATOM	2819	OH	TYR A 693	-9.721	8.651	-18.344	1.00	0.00
ATOM	2820	HN	TYR A 693	-14.562	9.956	-22.230	1.00	0.00
ATOM	2821	HA	TYR A 693	-14.054	11.149	-19.833	1.00	0.00
ATOM	2822	1HB	TYR A 693	-12.616	12.871	-21.396	1.00	0.00
ATOM	2823	2HB	TYR A 693	-12.937	11.603	-22.594	1.00	0.00
ATOM	2824	HD1	TYR A 693	-12.448	9.174	-21.902	1.00	0.00
ATOM	2825	HE1	TYR A 693	-11.046	7.760	-20.446	1.00	0.00
ATOM	2826	HD2	TYR A 693	-11.089	12.629	-19.830	1.00	0.00
ATOM	2827	HE2	TYR A 693	-9.643	11.233	-18.420	1.00	0.00
ATOM	2828	HH	TYR A 693	-9.926	9.002	-17.487	1.00	0.00
ATOM	2829	N	ILE A 694	-15.324	13.266	-22.084	1.00	0.00
ATOM	2830	CA	ILE A 694	-15.905	14.570	-22.166	1.00	0.00
ATOM	2831	C	ILE A 694	-17.151	14.605	-21.352	1.00	0.00
ATOM	2832	O	ILE A 694	-17.425	15.590	-20.668	1.00	0.00
ATOM	2833	CB	ILE A 694	-16.243	15.008	-23.564	1.00	0.00
ATOM	2834	CG1	ILE A 694	-16.539	16.517	-23.576	1.00	0.00
ATOM	2835	CG2	ILE A 694	-17.401	14.145	-24.087	1.00	0.00
ATOM	2836	CD1	ILE A 694	-16.577	17.126	-24.977	1.00	0.00
ATOM	2837	HN	ILE A 694	-15.214	12.701	-22.902	1.00	0.00
ATOM	2838	HA	ILE A 694	-15.179	15.256	-21.730	1.00	0.00
ATOM	2839	HB	ILE A 694	-15.373	14.893	-24.210	1.00	0.00
ATOM	2840	1HG2	ILE A 694	-18.314	14.734	-24.170	1.00	0.00
ATOM	2841	2HG2	ILE A 694	-17.595	13.319	-23.402	1.00	0.00

74/208

ATOM	2842	3HG2	ILE A 694	-17.162	13.753	-25.075	1.00	0.00
ATOM	2843	1HG1	ILE A 694	-15.771	17.028	-22.995	1.00	0.00
ATOM	2844	2HG1	ILE A 694	-17.502	16.688	-23.096	1.00	0.00
ATOM	2845	1HD1	ILE A 694	-17.351	16.652	-25.582	1.00	0.00
ATOM	2846	2HD1	ILE A 694	-15.621	16.978	-25.478	1.00	0.00
ATOM	2847	3HD1	ILE A 694	-16.801	18.191	-24.919	1.00	0.00
ATOM	2848	N	LYS A 695	-17.938	13.516	-21.384	1.00	0.00
ATOM	2849	CA	LYS A 695	-19.157	13.529	-20.639	1.00	0.00
ATOM	2850	C	LYS A 695	-18.843	13.722	-19.190	1.00	0.00
ATOM	2851	O	LYS A 695	-19.467	14.547	-18.523	1.00	0.00
ATOM	2852	CB	LYS A 695	-19.967	12.229	-20.781	1.00	0.00
ATOM	2853	CG	LYS A 695	-21.302	12.282	-20.036	1.00	0.00
ATOM	2854	CD	LYS A 695	-22.279	13.304	-20.617	1.00	0.00
ATOM	2855	CE	LYS A 695	-23.558	13.464	-19.793	1.00	0.00
ATOM	2856	NZ	LYS A 695	-23.266	14.222	-18.556	1.00	0.00
ATOM	2857	HN	LYS A 695	-17.674	12.713	-21.918	1.00	0.00
ATOM	2858	HA	LYS A 695	-19.739	14.373	-21.009	1.00	0.00
ATOM	2859	1HB	LYS A 695	-19.377	11.400	-20.390	1.00	0.00
ATOM	2860	2HB	LYS A 695	-20.158	12.045	-21.837	1.00	0.00
ATOM	2861	1HG	LYS A 695	-21.111	12.532	-18.993	1.00	0.00
ATOM	2862	2HG	LYS A 695	-21.763	11.296	-20.073	1.00	0.00
ATOM	2863	1HD	LYS A 695	-22.550	12.995	-21.626	1.00	0.00
ATOM	2864	2HD	LYS A 695	-21.780	14.270	-20.678	1.00	0.00
ATOM	2865	1HE	LYS A 695	-23.952	12.488	-19.510	1.00	0.00
ATOM	2866	2HE	LYS A 695	-24.310	14.013	-20.360	1.00	0.00
ATOM	2867	1HZ	LYS A 695	-22.898	15.162	-18.804	1.00	0.00
ATOM	2868	2HZ	LYS A 695	-22.557	13.709	-17.994	1.00	0.00
ATOM	2869	3HZ	LYS A 695	-24.139	14.328	-18.000	1.00	0.00
ATOM	2870	N	GLU A 696	-17.839	12.994	-18.659	1.00	0.00
ATOM	2871	CA	GLU A 696	-17.555	13.155	-17.265	1.00	0.00
ATOM	2872	C	GLU A 696	-17.124	14.559	-17.009	1.00	0.00
ATOM	2873	O	GLU A 696	-17.494	15.140	-15.989	1.00	0.00
ATOM	2874	CB	GLU A 696	-16.462	12.236	-16.677	1.00	0.00
ATOM	2875	CG	GLU A 696	-15.054	12.411	-17.246	1.00	0.00
ATOM	2876	CD	GLU A 696	-14.677	11.126	-17.965	1.00	0.00
ATOM	2877	OE1	GLU A 696	-15.592	10.298	-18.223	1.00	0.00
ATOM	2878	OE2	GLU A 696	-13.465	10.951	-18.262	1.00	0.00
ATOM	2879	HN	GLU A 696	-17.310	12.361	-19.224	1.00	0.00
ATOM	2880	HA	GLU A 696	-18.496	12.970	-16.749	1.00	0.00
ATOM	2881	1HB	GLU A 696	-16.766	11.204	-16.843	1.00	0.00
ATOM	2882	2HB	GLU A 696	-16.416	12.412	-15.604	1.00	0.00
ATOM	2883	1HG	GLU A 696	-14.338	12.600	-16.446	1.00	0.00
ATOM	2884	2HG	GLU A 696	-15.026	13.241	-17.952	1.00	0.00
ATOM	2885	N	LEU A 697	-16.332	15.163	-17.919	1.00	0.00
ATOM	2886	CA	LEU A 697	-15.923	16.501	-17.606	1.00	0.00
ATOM	2887	C	LEU A 697	-17.125	17.387	-17.521	1.00	0.00
ATOM	2888	O	LEU A 697	-17.223	18.217	-16.619	1.00	0.00
ATOM	2889	CB	LEU A 697	-14.934	17.177	-18.580	1.00	0.00
ATOM	2890	CG	LEU A 697	-13.522	16.555	-18.621	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

ATOM	2891	CD1	LEU A 697	-13.050	16.137	-17.219	1.00	0.00
ATOM	2892	CD2	LEU A 697	-13.367	15.482	-19.702	1.00	0.00
ATOM	2893	HN	LEU A 697	-16.049	14.705	-18.760	1.00	0.00
ATOM	2894	HA	LEU A 697	-15.468	16.443	-16.618	1.00	0.00
ATOM	2895	IHB	LEU A 697	-14.838	18.223	-18.297	1.00	0.00
ATOM	2896	2HB	LEU A 697	-15.357	17.129	-19.582	1.00	0.00
ATOM	2897	HG	LEU A 697	-12.821	17.280	-19.034	1.00	0.00
ATOM	2898	IHD1	LEU A 697	-13.342	15.109	-17.005	1.00	0.00
ATOM	2899	2HD1	LEU A 697	-13.501	16.780	-16.463	1.00	0.00
ATOM	2900	3HD1	LEU A 697	-11.964	16.199	-17.153	1.00	0.00
ATOM	2901	IHD2	LEU A 697	-12.720	15.834	-20.504	1.00	0.00
ATOM	2902	2HD2	LEU A 697	-14.338	15.241	-20.134	1.00	0.00
ATOM	2903	3HD2	LEU A 697	-12.921	14.583	-19.278	1.00	0.00
ATOM	2904	N	GLY A 698	-18.088	17.215	-18.447	1.00	0.00
ATOM	2905	CA	GLY A 698	-19.251	18.055	-18.451	1.00	0.00
ATOM	2906	C	GLY A 698	-19.965	17.888	-17.151	1.00	0.00
ATOM	2907	O	GLY A 698	-20.472	18.845	-16.571	1.00	0.00
ATOM	2908	HN	GLY A 698	-17.990	16.497	-19.136	1.00	0.00
ATOM	2909	IHA	GLY A 698	-19.891	17.744	-19.275	1.00	0.00
ATOM	2910	2HA	GLY A 698	-18.923	19.087	-18.571	1.00	0.00
ATOM	2911	N	LYS A 699	-20.020	16.646	-16.651	1.00	0.00
ATOM	2912	CA	LYS A 699	-20.696	16.400	-15.419	1.00	0.00
ATOM	2913	C	LYS A 699	-20.029	17.204	-14.345	1.00	0.00
ATOM	2914	O	LYS A 699	-20.701	17.796	-13.502	1.00	0.00
ATOM	2915	CB	LYS A 699	-20.667	14.897	-15.068	1.00	0.00
ATOM	2916	CG	LYS A 699	-21.365	14.527	-13.762	1.00	0.00
ATOM	2917	CD	LYS A 699	-20.564	14.961	-12.540	1.00	0.00
ATOM	2918	CE	LYS A 699	-21.431	15.484	-11.408	1.00	0.00
ATOM	2919	NZ	LYS A 699	-22.434	16.434	-11.943	1.00	0.00
ATOM	2920	HN	LYS A 699	-19.587	15.891	-17.143	1.00	0.00
ATOM	2921	HA	LYS A 699	-21.723	16.746	-15.540	1.00	0.00
ATOM	2922	IHB	LYS A 699	-19.628	14.581	-15.002	1.00	0.00
ATOM	2923	2HB	LYS A 699	-21.143	14.347	-15.879	1.00	0.00
ATOM	2924	IHG	LYS A 699	-21.509	13.448	-13.729	1.00	0.00
ATOM	2925	2HG	LYS A 699	-22.344	15.003	-13.734	1.00	0.00
ATOM	2926	IHD	LYS A 699	-19.867	15.744	-12.838	1.00	0.00
ATOM	2927	2HD	LYS A 699	-19.989	14.110	-12.178	1.00	0.00
ATOM	2928	IHE	LYS A 699	-20.821	16.009	-10.673	1.00	0.00
ATOM	2929	2HE	LYS A 699	-21.961	14.663	-10.925	1.00	0.00
ATOM	2930	1HZ	LYS A 699	-23.137	15.914	-12.508	1.00	0.00
ATOM	2931	2HZ	LYS A 699	-21.960	17.138	-12.543	1.00	0.00
ATOM	2932	3HZ	LYS A 699	-22.911	16.915	-11.154	1.00	0.00
ATOM	2933	N	ALA A 700	-18.684	17.255	-14.346	1.00	0.00
ATOM	2934	CA	ALA A 700	-17.988	17.961	-13.307	1.00	0.00
ATOM	2935	C	ALA A 700	-18.341	19.408	-13.349	1.00	0.00
ATOM	2936	O	ALA A 700	-18.623	20.018	-12.318	1.00	0.00
ATOM	2937	CB	ALA A 700	-16.460	17.857	-13.434	1.00	0.00
ATOM	2938	HN	ALA A 700	-18.169	16.801	-15.072	1.00	0.00
ATOM	2939	HA	ALA A 700	-18.316	17.528	-12.362	1.00	0.00

76/208

ATOM	2940	1HB	ALA	A	700	-16.123	18.273	-14.384	1.00	0.00
ATOM	2941	2HB	ALA	A	700	-16.149	16.813	-13.394	1.00	0.00
ATOM	2942	3HB	ALA	A	700	-15.976	18.415	-12.633	1.00	0.00
ATOM	2943	N	ILE	A	701	-18.351	19.996	-14.557	1.00	0.00
ATOM	2944	CA	ILE	A	701	-18.652	21.390	-14.648	1.00	0.00
ATOM	2945	C	ILE	A	701	-20.060	21.594	-14.212	1.00	0.00
ATOM	2946	O	ILE	A	701	-20.382	22.623	-13.631	1.00	0.00
ATOM	2947	CB	ILE	A	701	-18.482	21.972	-16.021	1.00	0.00
ATOM	2948	CG1	ILE	A	701	-19.449	21.343	-17.031	1.00	0.00
ATOM	2949	CG2	ILE	A	701	-17.004	21.821	-16.406	1.00	0.00
ATOM	2950	CD1	ILE	A	701	-19.478	22.085	-18.362	1.00	0.00
ATOM	2951	HN	ILE	A	701	-18.151	19.465	-15.380	1.00	0.00
ATOM	2952	HA	ILE	A	701	-17.982	21.892	-13.950	1.00	0.00
ATOM	2953	HB	ILE	A	701	-18.767	23.024	-16.024	1.00	0.00
ATOM	2954	1HG2	ILE	A	701	-16.712	20.771	-16.411	1.00	0.00
ATOM	2955	2HG2	ILE	A	701	-16.372	22.343	-15.688	1.00	0.00
ATOM	2956	3HG2	ILE	A	701	-16.832	22.222	-17.405	1.00	0.00
ATOM	2957	1HG1	ILE	A	701	-20.452	21.342	-16.605	1.00	0.00
ATOM	2958	2HG1	ILE	A	701	-19.152	20.310	-17.208	1.00	0.00
ATOM	2959	1HD1	ILE	A	701	-18.490	22.088	-18.823	1.00	0.00
ATOM	2960	2HD1	ILE	A	701	-19.781	23.121	-18.210	1.00	0.00
ATOM	2961	3HD1	ILE	A	701	-20.170	21.598	-19.050	1.00	0.00
ATOM	2962	N	VAL	A	702	-20.949	20.622	-14.475	1.00	0.00
ATOM	2963	CA	VAL	A	702	-22.319	20.788	-14.085	1.00	0.00
ATOM	2964	C	VAL	A	702	-22.425	20.931	-12.597	1.00	0.00
ATOM	2965	O	VAL	A	702	-23.157	21.790	-12.105	1.00	0.00
ATOM	2966	CB	VAL	A	702	-23.172	19.627	-14.482	1.00	0.00
ATOM	2967	CG1	VAL	A	702	-24.594	19.863	-13.944	1.00	0.00
ATOM	2968	CG2	VAL	A	702	-23.084	19.481	-16.010	1.00	0.00
ATOM	2969	HN	VAL	A	702	-20.656	19.787	-14.941	1.00	0.00
ATOM	2970	HA	VAL	A	702	-22.675	21.698	-14.568	1.00	0.00
ATOM	2971	HB	VAL	A	702	-22.764	18.705	-14.067	1.00	0.00
ATOM	2972	1HG1	VAL	A	702	-24.650	20.809	-13.406	1.00	0.00
ATOM	2973	2HG1	VAL	A	702	-24.873	19.066	-13.255	1.00	0.00
ATOM	2974	3HG1	VAL	A	702	-25.306	19.901	-14.769	1.00	0.00
ATOM	2975	1HG2	VAL	A	702	-22.197	19.983	-16.395	1.00	0.00
ATOM	2976	2HG2	VAL	A	702	-23.958	19.930	-16.482	1.00	0.00
ATOM	2977	3HG2	VAL	A	702	-23.021	18.428	-16.285	1.00	0.00
ATOM	2978	N	LYS	A	703	-21.685	20.107	-11.829	1.00	0.00
ATOM	2979	CA	LYS	A	703	-21.780	20.209	-10.397	1.00	0.00
ATOM	2980	C	LYS	A	703	-21.344	21.580	-10.022	1.00	0.00
ATOM	2981	O	LYS	A	703	-21.933	22.232	-9.161	1.00	0.00
ATOM	2982	CB	LYS	A	703	-20.815	19.297	-9.622	1.00	0.00
ATOM	2983	CG	LYS	A	703	-21.180	17.821	-9.655	1.00	0.00
ATOM	2984	CD	LYS	A	703	-20.112	16.900	-9.058	1.00	0.00
ATOM	2985	CE	LYS	A	703	-18.706	17.078	-9.634	1.00	0.00
ATOM	2986	NZ	LYS	A	703	-18.598	16.389	-10.938	1.00	0.00
ATOM	2987	HN	LYS	A	703	-21.077	19.434	-12.250	1.00	0.00
ATOM	2988	HA	LYS	A	703	-22.809	19.955	-10.143	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

77/208

ATOM	2989	1HB	LYS	A	703	-20.792	19.623	-8.583	1.00	0.00
ATOM	2990	2HB	LYS	A	703	-19.817	19.415	-10.041	1.00	0.00
ATOM	2991	1HG	LYS	A	703	-21.350	17.529	-10.691	1.00	0.00
ATOM	2992	2HG	LYS	A	703	-22.108	17.681	-9.103	1.00	0.00
ATOM	2993	1HD	LYS	A	703	-20.421	15.868	-9.220	1.00	0.00
ATOM	2994	2HD	LYS	A	703	-20.067	17.080	-7.985	1.00	0.00
ATOM	2995	1HE	LYS	A	703	-17.964	16.649	-8.961	1.00	0.00
ATOM	2996	2HE	LYS	A	703	-18.492	18.135	-9.790	1.00	0.00
ATOM	2997	1HZ	LYS	A	703	-19.292	16.791	-11.601	1.00	0.00
ATOM	2998	2HZ	LYS	A	703	-18.788	15.375	-10.811	1.00	0.00
ATOM	2999	3HZ	LYS	A	703	-17.639	16.517	-11.320	1.00	0.00
ATOM	3000	N	ARG	A	704	-20.273	22.026	-10.690	1.00	0.00
ATOM	3001	CA	ARG	A	704	-19.624	23.284	-10.496	1.00	0.00
ATOM	3002	C	ARG	A	704	-20.553	24.375	-10.917	1.00	0.00
ATOM	3003	O	ARG	A	704	-20.395	25.518	-10.507	1.00	0.00
ATOM	3004	CB	ARG	A	704	-18.371	23.420	-11.373	1.00	0.00
ATOM	3005	CG	ARG	A	704	-17.385	22.267	-11.197	1.00	0.00
ATOM	3006	CD	ARG	A	704	-16.448	22.425	-10.001	1.00	0.00
ATOM	3007	NE	ARG	A	704	-15.575	21.219	-9.975	1.00	0.00
ATOM	3008	CZ	ARG	A	704	-14.439	21.179	-10.732	1.00	0.00
ATOM	3009	NH1	ARG	A	704	-14.130	22.226	-11.549	1.00	0.00
ATOM	3010	NH2	ARG	A	704	-13.615	20.093	-10.666	1.00	0.00
ATOM	3011	HN	ARG	A	704	-19.893	21.422	-11.389	1.00	0.00
ATOM	3012	HA	ARG	A	704	-19.357	23.344	-9.441	1.00	0.00
ATOM	3013	1HB	ARG	A	704	-17.868	24.354	-11.123	1.00	0.00
ATOM	3014	2HB	ARG	A	704	-18.677	23.465	-12.417	1.00	0.00
ATOM	3015	1HG	ARG	A	704	-16.782	22.186	-12.100	1.00	0.00
ATOM	3016	2HG	ARG	A	704	-17.949	21.344	-11.076	1.00	0.00
ATOM	3017	1HD	ARG	A	704	-17.001	22.464	-9.064	1.00	0.00
ATOM	3018	2HD	ARG	A	704	-15.813	23.303	-10.105	1.00	0.00
ATOM	3019	HE	ARG	A	704	-15.820	20.437	-9.403	1.00	0.00
ATOM	3020	1HH1	ARG	A	704	-14.735	23.021	-11.593	1.00	0.00
ATOM	3021	2HH1	ARG	A	704	-13.299	22.198	-12.103	1.00	0.00
ATOM	3022	1HH2	ARG	A	704	-12.867	19.992	-11.323	1.00	0.00
ATOM	3023	2HH2	ARG	A	704	-13.759	19.398	-9.962	1.00	0.00
ATOM	3024	N	GLU	A	705	-21.526	24.047	-11.784	1.00	0.00
ATOM	3025	CA	GLU	A	705	-22.452	24.985	-12.346	1.00	0.00
ATOM	3026	C	GLU	A	705	-23.197	25.603	-11.225	1.00	0.00
ATOM	3027	O	GLU	A	705	-23.701	26.719	-11.350	1.00	0.00
ATOM	3028	CB	GLU	A	705	-23.467	24.326	-13.296	1.00	0.00
ATOM	3029	CG	GLU	A	705	-24.376	25.332	-14.004	1.00	0.00
ATOM	3030	CD	GLU	A	705	-23.519	26.124	-14.981	1.00	0.00
ATOM	3031	OE1	GLU	A	705	-23.147	27.278	-14.637	1.00	0.00
ATOM	3032	OE2	GLU	A	705	-23.216	25.584	-16.078	1.00	0.00
ATOM	3033	HN	GLU	A	705	-21.610	23.087	-12.052	1.00	0.00
ATOM	3034	HA	GLU	A	705	-21.859	25.724	-12.885	1.00	0.00
ATOM	3035	1HB	GLU	A	705	-24.086	23.637	-12.723	1.00	0.00
ATOM	3036	2HB	GLU	A	705	-22.924	23.755	-14.047	1.00	0.00
ATOM	3037	1HG	GLU	A	705	-24.829	26.014	-13.285	1.00	0.00

78/208

ATOM	3038	2HG	GLU	A	705	-25.166	24.816	-14.552	1.00	0.00
ATOM	3039	N	GLY	A	706	-23.302	24.865	-10.105	1.00	0.00
ATOM	3040	CA	GLY	A	706	-23.959	25.401	-8.954	1.00	0.00
ATOM	3041	C	GLY	A	706	-23.259	26.696	-8.655	1.00	0.00
ATOM	3042	O	GLY	A	706	-23.896	27.696	-8.328	1.00	0.00
ATOM	3043	HN	GLY	A	706	-22.920	23.941	-10.078	1.00	0.00
ATOM	3044	1HA	GLY	A	706	-23.850	24.701	-8.127	1.00	0.00
ATOM	3045	2HA	GLY	A	706	-25.007	25.573	-9.194	1.00	0.00
ATOM	3046	N	ASN	A	707	-21.914	26.694	-8.773	1.00	0.00
ATOM	3047	CA	ASN	A	707	-21.090	27.862	-8.605	1.00	0.00
ATOM	3048	C	ASN	A	707	-20.904	28.564	-9.933	1.00	0.00
ATOM	3049	O	ASN	A	707	-21.800	28.531	-10.775	1.00	0.00
ATOM	3050	CB	ASN	A	707	-19.699	27.572	-8.022	1.00	0.00
ATOM	3051	CG	ASN	A	707	-19.889	27.364	-6.528	1.00	0.00
ATOM	3052	OD1	ASN	A	707	-20.915	27.749	-5.970	1.00	0.00
ATOM	3053	ND2	ASN	A	707	-18.874	26.755	-5.859	1.00	0.00
ATOM	3054	HN	ASN	A	707	-21.465	25.829	-8.991	1.00	0.00
ATOM	3055	HA	ASN	A	707	-21.637	28.529	-7.940	1.00	0.00
ATOM	3056	1HB	ASN	A	707	-19.024	28.411	-8.192	1.00	0.00
ATOM	3057	2HB	ASN	A	707	-19.270	26.674	-8.466	1.00	0.00
ATOM	3058	1HD2	ASN	A	707	-18.885	26.730	-4.860	1.00	0.00
ATOM	3059	2HD2	ASN	A	707	-18.114	26.329	-6.349	1.00	0.00
ATOM	3060	N	SER	A	708	-19.744	29.240	-10.159	1.00	0.00
ATOM	3061	CA	SER	A	708	-19.586	29.964	-11.400	1.00	0.00
ATOM	3062	C	SER	A	708	-18.214	29.833	-12.019	1.00	0.00
ATOM	3063	O	SER	A	708	-17.723	28.727	-12.234	1.00	0.00
ATOM	3064	CB	SER	A	708	-19.894	31.469	-11.261	1.00	0.00
ATOM	3065	OG	SER	A	708	-19.957	32.087	-12.539	1.00	0.00
ATOM	3066	HN	SER	A	708	-19.014	29.235	-9.477	1.00	0.00
ATOM	3067	HA	SER	A	708	-20.268	29.507	-12.117	1.00	0.00
ATOM	3068	1HB	SER	A	708	-19.110	31.962	-10.685	1.00	0.00
ATOM	3069	2HB	SER	A	708	-20.854	31.613	-10.767	1.00	0.00
ATOM	3070	HG	SER	A	708	-20.537	31.556	-13.070	1.00	0.00
ATOM	3071	N	SER	A	709	-17.553	30.988	-12.286	1.00	0.00
ATOM	3072	CA	SER	A	709	-16.308	31.118	-13.009	1.00	0.00
ATOM	3073	C	SER	A	709	-15.219	30.341	-12.359	1.00	0.00
ATOM	3074	O	SER	A	709	-14.309	29.834	-13.014	1.00	0.00
ATOM	3075	CB	SER	A	709	-15.830	32.578	-13.122	1.00	0.00
ATOM	3076	OG	SER	A	709	-14.609	32.634	-13.845	1.00	0.00
ATOM	3077	HN	SER	A	709	-17.968	31.831	-11.950	1.00	0.00
ATOM	3078	HA	SER	A	709	-16.478	30.703	-14.002	1.00	0.00
ATOM	3079	1HB	SER	A	709	-15.661	32.998	-12.130	1.00	0.00
ATOM	3080	2HB	SER	A	709	-16.570	33.178	-13.651	1.00	0.00
ATOM	3081	HG	SER	A	709	-14.089	31.895	-13.560	1.00	0.00
ATOM	3082	N	GLN	A	710	-15.304	30.190	-11.034	1.00	0.00
ATOM	3083	CA	GLN	A	710	-14.320	29.451	-10.309	1.00	0.00
ATOM	3084	C	GLN	A	710	-14.284	28.076	-10.903	1.00	0.00
ATOM	3085	O	GLN	A	710	-13.284	27.368	-10.796	1.00	0.00
ATOM	3086	CB	GLN	A	710	-14.666	29.304	-8.816	1.00	0.00

SUBSTITUTE SHEET (RULE 26)



79/208

ATOM	3087	CG	GLN A 710	-14.694	30.629	-8.052	1.00	0.00
ATOM	3088	CD	GLN A 710	-15.988	31.361	-8.386	1.00	0.00
ATOM	3089	OE1	GLN A 710	-16.882	30.818	-9.034	1.00	0.00
ATOM	3090	NE2	GLN A 710	-16.096	32.635	-7.923	1.00	0.00
ATOM	3091	HN	GLN A 710	-16.071	30.602	-10.541	1.00	0.00
ATOM	3092	HA	GLN A 710	-13.378	29.988	-10.425	1.00	0.00
ATOM	3093	1HB	GLN A 710	-13.930	28.649	-8.352	1.00	0.00
ATOM	3094	2HB	GLN A 710	-15.645	28.833	-8.732	1.00	0.00
ATOM	3095	1HG	GLN A 710	-13.847	31.251	-8.341	1.00	0.00
ATOM	3096	2HG	GLN A 710	-14.653	30.448	-6.978	1.00	0.00
ATOM	3097	1HE2	GLN A 710	-15.346	33.036	-7.396	1.00	0.00
ATOM	3098	2HE2	GLN A 710	-16.913	33.183	-8.100	1.00	0.00
ATOM	3099	N	ASN A 711	-15.380	27.657	-11.559	1.00	0.00
ATOM	3100	CA	ASN A 711	-15.461	26.323	-12.067	1.00	0.00
ATOM	3101	C	ASN A 711	-14.298	25.993	-12.953	1.00	0.00
ATOM	3102	O	ASN A 711	-13.698	24.930	-12.804	1.00	0.00
ATOM	3103	CB	ASN A 711	-16.751	26.026	-12.870	1.00	0.00
ATOM	3104	CG	ASN A 711	-16.691	26.627	-14.274	1.00	0.00
ATOM	3105	OD1	ASN A 711	-16.897	25.908	-15.250	1.00	0.00
ATOM	3106	ND2	ASN A 711	-16.393	27.948	-14.394	1.00	0.00
ATOM	3107	HN	ASN A 711	-16.147	28.285	-11.693	1.00	0.00
ATOM	3108	HA	ASN A 711	-15.404	25.663	-11.202	1.00	0.00
ATOM	3109	1HB	ASN A 711	-17.611	26.448	-12.352	1.00	0.00
ATOM	3110	2HB	ASN A 711	-16.885	24.948	-12.964	1.00	0.00
ATOM	3111	1HD2	ASN A 711	-16.200	28.333	-15.296	1.00	0.00
ATOM	3112	2HD2	ASN A 711	-16.363	28.547	-13.594	1.00	0.00
ATOM	3113	N	TRP A 712	-13.916	26.884	-13.887	1.00	0.00
ATOM	3114	CA	TRP A 712	-12.853	26.497	-14.765	1.00	0.00
ATOM	3115	C	TRP A 712	-11.591	26.323	-13.993	1.00	0.00
ATOM	3116	O	TRP A 712	-10.832	25.390	-14.243	1.00	0.00
ATOM	3117	CB	TRP A 712	-12.619	27.465	-15.943	1.00	0.00
ATOM	3118	CG	TRP A 712	-12.309	28.896	-15.583	1.00	0.00
ATOM	3119	CD1	TRP A 712	-13.148	29.967	-15.494	1.00	0.00
ATOM	3120	CD2	TRP A 712	-10.988	29.388	-15.317	1.00	0.00
ATOM	3121	NE1	TRP A 712	-12.434	31.097	-15.174	1.00	0.00
ATOM	3122	CE2	TRP A 712	-11.101	30.754	-15.067	1.00	0.00
ATOM	3123	CE3	TRP A 712	-9.779	28.754	-15.292	1.00	0.00
ATOM	3124	CZ2	TRP A 712	-10.001	31.512	-14.785	1.00	0.00
ATOM	3125	CZ3	TRP A 712	-8.671	29.521	-15.011	1.00	0.00
ATOM	3126	CH2	TRP A 712	-8.781	30.873	-14.762	1.00	0.00
ATOM	3127	HN	TRP A 712	-14.356	27.778	-13.963	1.00	0.00
ATOM	3128	HA	TRP A 712	-13.116	25.510	-15.145	1.00	0.00
ATOM	3129	1HB	TRP A 712	-13.514	27.473	-16.563	1.00	0.00
ATOM	3130	2HB	TRP A 712	-11.783	27.091	-16.532	1.00	0.00
ATOM	3131	HE3	TRP A 712	-9.696	27.695	-15.485	1.00	0.00
ATOM	3132	HD1	TRP A 712	-14.216	29.933	-15.652	1.00	0.00
ATOM	3133	HE1	TRP A 712	-12.807	31.993	-15.043	1.00	0.00
ATOM	3134	HZ2	TRP A 712	-10.084	32.570	-14.587	1.00	0.00
ATOM	3135	HZ3	TRP A 712	-7.697	29.055	-14.985	1.00	0.00

80/208

ATOM	3136	HH2 TRP A 712	-7.891	31.444	-14.544	1.00	0.00
ATOM	3137	N GLN A 713	-11.330	27.211	-13.017	1.00	0.00
ATOM	3138	CA GLN A 713	-10.107	27.075	-12.282	1.00	0.00
ATOM	3139	C GLN A 713	-10.089	25.802	-11.491	1.00	0.00
ATOM	3140	O GLN A 713	-9.093	25.080	-11.508	1.00	0.00
ATOM	3141	CB GLN A 713	-9.821	28.261	-11.342	1.00	0.00
ATOM	3142	CG GLN A 713	-10.838	28.460	-10.220	1.00	0.00
ATOM	3143	CD GLN A 713	-10.394	29.664	-9.403	1.00	0.00
ATOM	3144	OE1 GLN A 713	-9.241	29.755	-8.985	1.00	0.00
ATOM	3145	NE2 GLN A 713	-11.331	30.626	-9.180	1.00	0.00
ATOM	3146	HN GLN A 713	-11.973	27.947	-12.809	1.00	0.00
ATOM	3147	HA GLN A 713	-9.311	26.985	-13.021	1.00	0.00
ATOM	3148	IHB GLN A 713	-9.789	29.171	-11.939	1.00	0.00
ATOM	3149	2HB GLN A 713	-8.840	28.112	-10.892	1.00	0.00
ATOM	3150	IHG GLN A 713	-10.877	27.581	-9.577	1.00	0.00
ATOM	3151	2HG GLN A 713	-11.830	28.646	-10.630	1.00	0.00
ATOM	3152	IHE2 GLN A 713	-12.287	30.451	-9.415	1.00	0.00
ATOM	3153	2HE2 GLN A 713	-11.082	31.509	-8.783	1.00	0.00
ATOM	3154	N ARG A 714	-11.197	25.461	-10.801	1.00	0.00
ATOM	3155	CA ARG A 714	-11.173	24.266	-10.001	1.00	0.00
ATOM	3156	C ARG A 714	-10.968	23.072	-10.861	1.00	0.00
ATOM	3157	O ARG A 714	-10.272	22.135	-10.473	1.00	0.00
ATOM	3158	CB ARG A 714	-12.450	23.958	-9.200	1.00	0.00
ATOM	3159	CG ARG A 714	-12.332	22.584	-8.521	1.00	0.00
ATOM	3160	CD ARG A 714	-13.646	21.995	-8.004	1.00	0.00
ATOM	3161	NE ARG A 714	-13.923	22.565	-6.658	1.00	0.00
ATOM	3162	CZ ARG A 714	-13.668	21.828	-5.538	1.00	0.00
ATOM	3163	NH1 ARG A 714	-13.907	22.359	-4.303	1.00	0.00
ATOM	3164	NH2 ARG A 714	-13.186	20.556	-5.651	1.00	0.00
ATOM	3165	HN ARG A 714	-12.019	26.028	-10.846	1.00	0.00
ATOM	3166	HA ARG A 714	-10.337	24.388	-9.313	1.00	0.00
ATOM	3167	IHB ARG A 714	-13.310	23.963	-9.869	1.00	0.00
ATOM	3168	2HB ARG A 714	-12.601	24.728	-8.443	1.00	0.00
ATOM	3169	IHG ARG A 714	-11.647	22.677	-7.680	1.00	0.00
ATOM	3170	2HG ARG A 714	-11.905	21.885	-9.238	1.00	0.00
ATOM	3171	IHD ARG A 714	-13.576	20.913	-7.899	1.00	0.00
ATOM	3172	2HD ARG A 714	-14.478	22.260	-8.656	1.00	0.00
ATOM	3173	HE ARG A 714	-14.297	23.489	-6.573	1.00	0.00
ATOM	3174	IHH1 ARG A 714	-14.268	23.288	-4.219	1.00	0.00
ATOM	3175	2HH1 ARG A 714	-13.720	21.819	-3.482	1.00	0.00
ATOM	3176	IHH2 ARG A 714	-12.724	20.126	-4.876	1.00	0.00
ATOM	3177	2HH2 ARG A 714	-13.296	20.054	-6.509	1.00	0.00
ATOM	3178	N PHE A 715	-11.573	23.082	-12.059	1.00	0.00
ATOM	3179	CA PHE A 715	-11.501	21.952	-12.932	1.00	0.00
ATOM	3180	C PHE A 715	-10.049	21.682	-13.163	1.00	0.00
ATOM	3181	O PHE A 715	-9.574	20.558	-12.995	1.00	0.00
ATOM	3182	CB PHE A 715	-12.180	22.267	-14.278	1.00	0.00
ATOM	3183	CG PHE A 715	-12.190	21.056	-15.138	1.00	0.00
ATOM	3184	CD1 PHE A 715	-11.089	20.730	-15.896	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

81/208

ATOM	3185	CD2 PHE A 715	-13.348	20.329	-15.286	1.00	0.00
ATOM	3186	CE1 PHE A 715	-11.142	19.685	-16.784	1.00	0.00
ATOM	3187	CE2 PHE A 715	-13.406	19.282	-16.173	1.00	0.00
ATOM	3188	CZ PHE A 715	-12.305	18.969	-16.931	1.00	0.00
ATOM	3189	HN PHE A 715	-12.083	23.893	-12.345	1.00	0.00
ATOM	3190	HA PHE A 715	-12.003	21.124	-12.432	1.00	0.00
ATOM	3191	IHB PHE A 715	-11.639	23.063	-14.790	1.00	0.00
ATOM	3192	2HB PHE A 715	-13.207	22.591	-14.109	1.00	0.00
ATOM	3193	HD1 PHE A 715	-10.178	21.300	-15.792	1.00	0.00
ATOM	3194	HD2 PHE A 715	-14.219	20.583	-14.700	1.00	0.00
ATOM	3195	HE1 PHE A 715	-10.271	19.426	-17.367	1.00	0.00
ATOM	3196	HE2 PHE A 715	-14.315	18.707	-16.273	1.00	0.00
ATOM	3197	HZ PHE A 715	-12.353	18.159	-17.643	1.00	0.00
ATOM	3198	N TYR A 716	-9.289	22.737	-13.493	1.00	0.00
ATOM	3199	CA TYR A 716	-7.900	22.550	-13.770	1.00	0.00
ATOM	3200	C TYR A 716	-7.194	22.064	-12.541	1.00	0.00
ATOM	3201	O TYR A 716	-6.394	21.132	-12.613	1.00	0.00
ATOM	3202	CB TYR A 716	-7.222	23.842	-14.256	1.00	0.00
ATOM	3203	CG TYR A 716	-5.825	23.506	-14.644	1.00	0.00
ATOM	3204	CD1 TYR A 716	-5.581	22.804	-15.802	1.00	0.00
ATOM	3205	CD2 TYR A 716	-4.758	23.997	-13.927	1.00	0.00
ATOM	3206	CE1 TYR A 716	-4.294	22.552	-16.214	1.00	0.00
ATOM	3207	CE2 TYR A 716	-3.468	23.756	-14.339	1.00	0.00
ATOM	3208	CZ TYR A 716	-3.235	23.028	-15.481	1.00	0.00
ATOM	3209	OH TYR A 716	-1.912	22.781	-15.905	1.00	0.00
ATOM	3210	HN TYR A 716	-9.693	23.650	-13.544	1.00	0.00
ATOM	3211	HA TYR A 716	-7.833	21.779	-14.537	1.00	0.00
ATOM	3212	IHB TYR A 716	-7.211	24.589	-13.462	1.00	0.00
ATOM	3213	2HB TYR A 716	-7.751	24.251	-15.116	1.00	0.00
ATOM	3214	HD1 TYR A 716	-6.411	22.446	-16.394	1.00	0.00
ATOM	3215	HE1 TYR A 716	-4.116	21.980	-17.113	1.00	0.00
ATOM	3216	HD2 TYR A 716	-4.936	24.578	-13.034	1.00	0.00
ATOM	3217	HE2 TYR A 716	-2.638	24.140	-13.764	1.00	0.00
ATOM	3218	HH TYR A 716	-1.407	22.435	-15.181	1.00	0.00
ATOM	3219	N GLN A 717	-7.480	22.658	-11.365	1.00	0.00
ATOM	3220	CA GLN A 717	-6.767	22.208	-10.203	1.00	0.00
ATOM	3221	C GLN A 717	-7.093	20.799	-9.825	1.00	0.00
ATOM	3222	O GLN A 717	-6.242	20.068	-9.319	1.00	0.00
ATOM	3223	CB GLN A 717	-6.848	23.111	-8.952	1.00	0.00
ATOM	3224	CG GLN A 717	-8.239	23.434	-8.409	1.00	0.00
ATOM	3225	CD GLN A 717	-8.473	24.912	-8.692	1.00	0.00
ATOM	3226	OE1 GLN A 717	-9.459	25.503	-8.254	1.00	0.00
ATOM	3227	NE2 GLN A 717	-7.511	25.541	-9.419	1.00	0.00
ATOM	3228	HN GLN A 717	-8.165	23.384	-11.305	1.00	0.00
ATOM	3229	HA GLN A 717	-5.726	22.118	-10.514	1.00	0.00
ATOM	3230	IHB GLN A 717	-6.359	24.053	-9.192	1.00	0.00
ATOM	3231	2HB GLN A 717	-6.287	22.625	-8.156	1.00	0.00
ATOM	3232	IHG GLN A 717	-8.292	23.251	-7.336	1.00	0.00
ATOM	3233	2HG GLN A 717	-9.002	22.838	-8.910	1.00	0.00

82/208

ATOM	3234	1HE2	GLN	A	717	-7.086	25.069	-10.191	1.00	0.00
ATOM	3235	2HE2	GLN	A	717	-7.218	26.470	-9.196	1.00	0.00
ATOM	3236	N	LEU	A	718	-8.345	20.378	-10.043	1.00	0.00
ATOM	3237	CA	LEU	A	718	-8.759	19.061	-9.662	1.00	0.00
ATOM	3238	C	LEU	A	718	-7.997	18.065	-10.503	1.00	0.00
ATOM	3239	O	LEU	A	718	-7.428	17.099	-9.995	1.00	0.00
ATOM	3240	CB	LEU	A	718	-10.288	18.979	-9.871	1.00	0.00
ATOM	3241	CG	LEU	A	718	-11.062	17.937	-9.047	1.00	0.00
ATOM	3242	CD1	LEU	A	718	-10.887	16.514	-9.571	1.00	0.00
ATOM	3243	CD2	LEU	A	718	-10.734	18.069	-7.552	1.00	0.00
ATOM	3244	HN	LEU	A	718	-9.000	20.994	-10.479	1.00	0.00
ATOM	3245	HA	LEU	A	718	-8.493	18.913	-8.616	1.00	0.00
ATOM	3246	1HB	LEU	A	718	-10.466	18.767	-10.923	1.00	0.00
ATOM	3247	2HB	LEU	A	718	-10.705	19.958	-9.640	1.00	0.00
ATOM	3248	HG	LEU	A	718	-12.122	18.190	-9.065	1.00	0.00
ATOM	3249	1HD1	LEU	A	718	-9.911	16.395	-10.041	1.00	0.00
ATOM	3250	2HD1	LEU	A	718	-11.650	16.290	-10.315	1.00	0.00
ATOM	3251	3HD1	LEU	A	718	-10.955	15.800	-8.750	1.00	0.00
ATOM	3252	1HD2	LEU	A	718	-10.835	19.104	-7.226	1.00	0.00
ATOM	3253	2HD2	LEU	A	718	-9.708	17.754	-7.363	1.00	0.00
ATOM	3254	3HD2	LEU	A	718	-11.419	17.461	-6.962	1.00	0.00
ATOM	3255	N	THR	A	719	-7.913	18.326	-11.823	1.00	0.00
ATOM	3256	CA	THR	A	719	-7.266	17.449	-12.761	1.00	0.00
ATOM	3257	C	THR	A	719	-5.793	17.323	-12.512	1.00	0.00
ATOM	3258	O	THR	A	719	-5.244	16.230	-12.641	1.00	0.00
ATOM	3259	CB	THR	A	719	-7.433	17.911	-14.178	1.00	0.00
ATOM	3260	OG1	THR	A	719	-6.820	19.179	-14.356	1.00	0.00
ATOM	3261	CG2	THR	A	719	-8.936	18.002	-14.489	1.00	0.00
ATOM	3262	HN	THR	A	719	-8.322	19.171	-12.167	1.00	0.00
ATOM	3263	HA	THR	A	719	-7.712	16.463	-12.630	1.00	0.00
ATOM	3264	HB	THR	A	719	-6.963	17.206	-14.864	1.00	0.00
ATOM	3265	HG1	THR	A	719	-5.901	19.069	-14.148	1.00	0.00
ATOM	3266	1HG2	THR	A	719	-9.482	18.409	-13.638	1.00	0.00
ATOM	3267	2HG2	THR	A	719	-9.337	17.011	-14.704	1.00	0.00
ATOM	3268	3HG2	THR	A	719	-9.105	18.658	-15.343	1.00	0.00
ATOM	3269	N	LYS	A	720	-5.093	18.417	-12.150	1.00	0.00
ATOM	3270	CA	LYS	A	720	-3.672	18.243	-12.010	1.00	0.00
ATOM	3271	C	LYS	A	720	-3.334	17.332	-10.872	1.00	0.00
ATOM	3272	O	LYS	A	720	-2.267	16.722	-10.867	1.00	0.00
ATOM	3273	CB	LYS	A	720	-2.780	19.505	-11.921	1.00	0.00
ATOM	3274	CG	LYS	A	720	-2.797	20.308	-10.622	1.00	0.00
ATOM	3275	CD	LYS	A	720	-4.022	21.194	-10.462	1.00	0.00
ATOM	3276	CE	LYS	A	720	-4.127	22.275	-11.542	1.00	0.00
ATOM	3277	NZ	LYS	A	720	-2.912	23.122	-11.534	1.00	0.00
ATOM	3278	HN	LYS	A	720	-5.536	19.298	-11.988	1.00	0.00
ATOM	3279	HA	LYS	A	720	-3.369	17.661	-12.880	1.00	0.00
ATOM	3280	1HB	LYS	A	720	-3.081	20.175	-12.723	1.00	0.00
ATOM	3281	2HB	LYS	A	720	-1.753	19.192	-12.098	1.00	0.00
ATOM	3282	1HG	LYS	A	720	-1.907	20.935	-10.590	1.00	0.00

83/208

ATOM 3283 2HG LYS A 720	-2.757	19.614	-9.784	1.00	0.00
ATOM 3284 1HD LYS A 720	-3.982	21.675	-9.485	1.00	0.00
ATOM 3285 2HD LYS A 720	-4.914	20.570	-10.501	1.00	0.00
ATOM 3286 1HE LYS A 720	-4.989	22.916	-11.355	1.00	0.00
ATOM 3287 2HE LYS A 720	-4.216	21.819	-12.528	1.00	0.00
ATOM 3288 1HZ LYS A 720	-2.077	22.532	-11.722	1.00	0.00
ATOM 3289 2HZ LYS A 720	-2.813	23.577	-10.604	1.00	0.00
ATOM 3290 3HZ LYS A 720	-2.993	23.852	-12.270	1.00	0.00
ATOM 3291 N LEU A 721	-4.227	17.216	-9.873	1.00	0.00
ATOM 3292 CA LEU A 721	-3.978	16.374	-8.733	1.00	0.00
ATOM 3293 C LEU A 721	-3.756	14.989	-9.260	1.00	0.00
ATOM 3294 O LEU A 721	-2.949	14.229	-8.726	1.00	0.00
ATOM 3295 CB LEU A 721	-5.180	16.384	-7.757	1.00	0.00
ATOM 3296 CG LEU A 721	-5.050	15.608	-6.423	1.00	0.00
ATOM 3297 CD1 LEU A 721	-6.341	15.751	-5.601	1.00	0.00
ATOM 3298 CD2 LEU A 721	-4.679	14.127	-6.606	1.00	0.00
ATOM 3299 HN LEU A 721	-5.085	17.728	-9.924	1.00	0.00
ATOM 3300 HA LEU A 721	-3.084	16.757	-8.241	1.00	0.00
ATOM 3301 1HB LEU A 721	-6.036	15.975	-8.290	1.00	0.00
ATOM 3302 2HB LEU A 721	-5.391	17.423	-7.510	1.00	0.00
ATOM 3303 HG LEU A 721	-4.208	15.999	-5.853	1.00	0.00
ATOM 3304 1HD1 LEU A 721	-7.158	15.200	-6.068	1.00	0.00
ATOM 3305 2HD1 LEU A 721	-6.634	16.799	-5.538	1.00	0.00
ATOM 3306 3HD1 LEU A 721	-6.195	15.350	-4.598	1.00	0.00
ATOM 3307 1HD2 LEU A 721	-3.597	13.999	-6.607	1.00	0.00
ATOM 3308 2HD2 LEU A 721	-5.064	13.757	-7.556	1.00	0.00
ATOM 3309 3HD2 LEU A 721	-5.088	13.534	-5.788	1.00	0.00
ATOM 3310 N LEU A 722	-4.443	14.633	-10.356	1.00	0.00
ATOM 3311 CA LEU A 722	-4.320	13.307	-10.888	1.00	0.00
ATOM 3312 C LEU A 722	-2.887	13.009	-11.191	1.00	0.00
ATOM 3313 O LEU A 722	-2.442	11.872	-11.040	1.00	0.00
ATOM 3314 CB LEU A 722	-5.125	13.093	-12.177	1.00	0.00
ATOM 3315 CG LEU A 722	-6.645	13.143	-11.952	1.00	0.00
ATOM 3316 CD1 LEU A 722	-7.109	14.534	-11.493	1.00	0.00
ATOM 3317 CD2 LEU A 722	-7.396	12.646	-13.191	1.00	0.00
ATOM 3318 HN LEU A 722	-5.044	15.296	-10.804	1.00	0.00
ATOM 3319 HA LEU A 722	-4.672	12.628	-10.111	1.00	0.00
ATOM 3320 1HB LEU A 722	-4.863	12.123	-12.598	1.00	0.00
ATOM 3321 2HB LEU A 722	-4.850	13.864	-12.895	1.00	0.00
ATOM 3322 HG LEU A 722	-6.920	12.407	-11.197	1.00	0.00
ATOM 3323 1HD1 LEU A 722	-6.709	15.309	-12.147	1.00	0.00
ATOM 3324 2HD1 LEU A 722	-6.756	14.733	-10.481	1.00	0.00
ATOM 3325 3HD1 LEU A 722	-8.196	14.597	-11.521	1.00	0.00
ATOM 3326 1HD2 LEU A 722	-6.803	11.906	-13.729	1.00	0.00
ATOM 3327 2HD2 LEU A 722	-7.595	13.476	-13.869	1.00	0.00
ATOM 3328 3HD2 LEU A 722	-8.336	12.178	-12.899	1.00	0.00
ATOM 3329 N ASP A 723	-2.119	14.019	-11.633	1.00	0.00
ATOM 3330 CA ASP A 723	-0.741	13.792	-11.962	1.00	0.00
ATOM 3331 C ASP A 723	-0.010	13.274	-10.759	1.00	0.00

84/208

ATOM 3332 O ASP A 723	0.743	12.305	-10.854	1.00	0.00
ATOM 3333 CB ASP A 723	-0.030	15.083	-12.405	1.00	0.00
ATOM 3334 CG ASP A 723	1.370	14.732	-12.890	1.00	0.00
ATOM 3335 OD1 ASP A 723	2.107	15.674	-13.288	1.00	0.00
ATOM 3336 OD2 ASP A 723	1.720	13.522	-12.876	1.00	0.00
ATOM 3337 HN ASP A 723	-2.510	14.934	-11.733	1.00	0.00
ATOM 3338 HA ASP A 723	-0.725	13.057	-12.767	1.00	0.00
ATOM 3339 1HB ASP A 723	0.047	15.779	-11.569	1.00	0.00
ATOM 3340 2HB ASP A 723	-0.580	15.560	-13.216	1.00	0.00
ATOM 3341 N SER A 724	-0.232	13.895	-9.585	1.00	0.00
ATOM 3342 CA SER A 724	0.455	13.494	-8.388	1.00	0.00
ATOM 3343 C SER A 724	0.075	12.088	-8.070	1.00	0.00
ATOM 3344 O SER A 724	0.909	11.279	-7.664	1.00	0.00
ATOM 3345 CB SER A 724	0.076	14.348	-7.166	1.00	0.00
ATOM 3346 OG SER A 724	0.481	15.694	-7.363	1.00	0.00
ATOM 3347 HN SER A 724	-0.888	14.649	-9.546	1.00	0.00
ATOM 3348 HA SER A 724	1.521	13.587	-8.595	1.00	0.00
ATOM 3349 1HB SER A 724	0.573	13.970	-6.273	1.00	0.00
ATOM 3350 2HB SER A 724	-1.003	14.336	-7.016	1.00	0.00
ATOM 3351 HG SER A 724	1.389	15.668	-7.634	1.00	0.00
ATOM 3352 N MET A 725	-1.212	11.757	-8.261	1.00	0.00
ATOM 3353 CA MET A 725	-1.668	10.440	-7.944	1.00	0.00
ATOM 3354 C MET A 725	-0.915	9.461	-8.785	1.00	0.00
ATOM 3355 O MET A 725	-0.510	8.408	-8.298	1.00	0.00
ATOM 3356 CB MET A 725	-3.164	10.256	-8.196	1.00	0.00
ATOM 3357 CG MET A 725	-4.058	11.063	-7.257	1.00	0.00
ATOM 3358 SD MET A 725	-5.826	10.823	-7.583	1.00	0.00
ATOM 3359 CE MET A 725	-5.715	9.033	-7.303	1.00	0.00
ATOM 3360 HN MET A 725	-1.852	12.434	-8.625	1.00	0.00
ATOM 3361 HA MET A 725	-1.441	10.276	-6.890	1.00	0.00
ATOM 3362 1HB MET A 725	-3.408	9.200	-8.083	1.00	0.00
ATOM 3363 2HB MET A 725	-3.382	10.551	-9.221	1.00	0.00
ATOM 3364 1HG MET A 725	-3.832	12.123	-7.370	1.00	0.00
ATOM 3365 2HG MET A 725	-3.858	10.767	-6.228	1.00	0.00
ATOM 3366 1HE MET A 725	-5.897	8.818	-6.250	1.00	0.00
ATOM 3367 2HE MET A 725	-4.719	8.677	-7.564	1.00	0.00
ATOM 3368 3HE MET A 725	-6.469	8.517	-7.898	1.00	0.00
ATOM 3369 N HIS A 726	-0.694	9.788	-10.072	1.00	0.00
ATOM 3370 CA HIS A 726	0.036	8.910	-10.943	1.00	0.00
ATOM 3371 C HIS A 726	1.424	8.772	-10.390	1.00	0.00
ATOM 3372 O HIS A 726	2.024	7.699	-10.419	1.00	0.00
ATOM 3373 CB HIS A 726	0.161	9.465	-12.373	1.00	0.00
ATOM 3374 CG HIS A 726	0.837	8.528	-13.331	1.00	0.00
ATOM 3375 ND1 HIS A 726	0.193	7.499	-13.981	1.00	0.00
ATOM 3376 CD2 HIS A 726	2.124	8.498	-13.772	1.00	0.00
ATOM 3377 CE1 HIS A 726	1.115	6.900	-14.777	1.00	0.00
ATOM 3378 NE2 HIS A 726	2.302	7.471	-14.685	1.00	0.00
ATOM 3379 HN HIS A 726	-1.044	10.655	-10.426	1.00	0.00
ATOM 3380 HA HIS A 726	-0.500	7.962	-10.953	1.00	0.00

85/208

ATOM 3381	IHB HIS A 726	0.734	10.391	-12.345	1.00	0.00
ATOM 3382	2HB HIS A 726	-0.836	9.679	-12.758	1.00	0.00
ATOM 3383	HD2 HIS A 726	2.899	9.179	-13.455	1.00	0.00
ATOM 3384	HD1 HIS A 726	-0.750	7.247	-13.886	1.00	0.00
ATOM 3385	HE1 HIS A 726	0.903	6.054	-15.412	1.00	0.00
ATOM 3386	N GLU A 727	1.986	9.871	-9.863	1.00	0.00
ATOM 3387	CA GLU A 727	3.321	9.790	-9.352	1.00	0.00
ATOM 3388	C GLU A 727	3.378	8.829	-8.205	1.00	0.00
ATOM 3389	O GLU A 727	4.243	7.955	-8.158	1.00	0.00
ATOM 3390	CB GLU A 727	3.841	11.150	-8.853	1.00	0.00
ATOM 3391	CG GLU A 727	5.295	11.127	-8.376	1.00	0.00
ATOM 3392	CD GLU A 727	5.332	10.686	-6.918	1.00	0.00
ATOM 3393	OE1 GLU A 727	6.457	10.435	-6.410	1.00	0.00
ATOM 3394	OE2 GLU A 727	4.242	10.600	-6.293	1.00	0.00
ATOM 3395	HN GLU A 727	1.479	10.733	-9.827	1.00	0.00
ATOM 3396	HA GLU A 727	3.947	9.424	-10.166	1.00	0.00
ATOM 3397	IHB GLU A 727	3.211	11.481	-8.028	1.00	0.00
ATOM 3398	2HB GLU A 727	3.754	11.873	-9.663	1.00	0.00
ATOM 3399	IHG GLU A 727	5.736	12.121	-8.458	1.00	0.00
ATOM 3400	2HG GLU A 727	5.879	10.428	-8.974	1.00	0.00
ATOM 3401	N VAL A 728	2.426	8.949	-7.260	1.00	0.00
ATOM 3402	CA VAL A 728	2.421	8.126	-6.084	1.00	0.00
ATOM 3403	C VAL A 728	2.245	6.693	-6.460	1.00	0.00
ATOM 3404	O VAL A 728	2.901	5.819	-5.893	1.00	0.00
ATOM 3405	CB VAL A 728	1.307	8.467	-5.137	1.00	0.00
ATOM 3406	CG1 VAL A 728	1.343	7.471	-3.965	1.00	0.00
ATOM 3407	CG2 VAL A 728	1.458	9.936	-4.705	1.00	0.00
ATOM 3408	HN VAL A 728	1.704	9.629	-7.382	1.00	0.00
ATOM 3409	HA VAL A 728	3.385	8.272	-5.597	1.00	0.00
ATOM 3410	HB VAL A 728	0.348	8.405	-5.650	1.00	0.00
ATOM 3411	IHG1 VAL A 728	2.370	7.266	-3.664	1.00	0.00
ATOM 3412	2HG1 VAL A 728	0.883	6.527	-4.259	1.00	0.00
ATOM 3413	3HG1 VAL A 728	0.816	7.883	-3.104	1.00	0.00
ATOM 3414	IHG2 VAL A 728	1.409	10.598	-5.570	1.00	0.00
ATOM 3415	2HG2 VAL A 728	2.420	10.088	-4.217	1.00	0.00
ATOM 3416	3HG2 VAL A 728	0.653	10.212	-4.023	1.00	0.00
ATOM 3417	N VAL A 729	1.351	6.419	-7.432	1.00	0.00
ATOM 3418	CA VAL A 729	1.114	5.066	-7.846	1.00	0.00
ATOM 3419	C VAL A 729	2.347	4.436	-8.386	1.00	0.00
ATOM 3420	O VAL A 729	2.634	3.280	-8.079	1.00	0.00
ATOM 3421	CB VAL A 729	0.025	4.898	-8.881	1.00	0.00
ATOM 3422	CG1 VAL A 729	-0.103	6.135	-9.771	1.00	0.00
ATOM 3423	CG2 VAL A 729	0.399	3.659	-9.717	1.00	0.00
ATOM 3424	HN VAL A 729	0.849	7.166	-7.868	1.00	0.00
ATOM 3425	HA VAL A 729	0.849	4.516	-6.943	1.00	0.00
ATOM 3426	HB VAL A 729	-0.924	4.719	-8.377	1.00	0.00
ATOM 3427	IHG1 VAL A 729	0.243	5.920	-10.781	1.00	0.00
ATOM 3428	2HG1 VAL A 729	0.502	6.949	-9.373	1.00	0.00
ATOM 3429	3HG1 VAL A 729	-1.145	6.449	-9.831	1.00	0.00

86/208

ATOM 3430 IHG2 VAL A 729	0.802	2.871	-9.080	1.00	0.00
ATOM 3431 2HG2 VAL A 729	1.160	3.918	-10.454	1.00	0.00
ATOM 3432 3HG2 VAL A 729	-0.482	3.266	-10.223	1.00	0.00
ATOM 3433 N GLU A 730	3.121	5.177	-9.194	1.00	0.00
ATOM 3434 CA GLU A 730	4.298	4.583	-9.753	1.00	0.00
ATOM 3435 C GLU A 730	5.209	4.190	-8.637	1.00	0.00
ATOM 3436 O GLU A 730	5.754	3.088	-8.626	1.00	0.00
ATOM 3437 CB GLU A 730	5.081	5.542	-10.669	1.00	0.00
ATOM 3438 CG GLU A 730	4.352	5.894	-11.968	1.00	0.00
ATOM 3439 CD GLU A 730	5.250	6.829	-12.770	1.00	0.00
ATOM 3440 OE1 GLU A 730	4.873	7.167	-13.923	1.00	0.00
ATOM 3441 OE2 GLU A 730	6.327	7.211	-12.241	1.00	0.00
ATOM 3442 HN GLU A 730	2.880	6.125	-9.400	1.00	0.00
ATOM 3443 HA GLU A 730	3.967	3.712	-10.319	1.00	0.00
ATOM 3444 1HB GLU A 730	6.035	5.080	-10.920	1.00	0.00
ATOM 3445 2HB GLU A 730	5.278	6.462	-10.121	1.00	0.00
ATOM 3446 1HG GLU A 730	3.408	6.395	-11.755	1.00	0.00
ATOM 3447 2HG GLU A 730	4.154	4.995	-12.552	1.00	0.00
ATOM 3448 N ASN A 731	5.383	5.085	-7.649	1.00	0.00
ATOM 3449 CA ASN A 731	6.262	4.803	-6.553	1.00	0.00
ATOM 3450 C ASN A 731	5.724	3.642	-5.785	1.00	0.00
ATOM 3451 O ASN A 731	6.482	2.778	-5.346	1.00	0.00
ATOM 3452 CB ASN A 731	6.391	5.978	-5.566	1.00	0.00
ATOM 3453 CG ASN A 731	7.092	7.133	-6.272	1.00	0.00
ATOM 3454 OD1 ASN A 731	6.004	6.959	-5.719	1.00	0.00
ATOM 3455 ND2 ASN A 731	8.213	6.414	-6.535	1.00	0.00
ATOM 3456 HN ASN A 731	4.894	5.957	-7.679	1.00	0.00
ATOM 3457 HA ASN A 731	7.235	4.570	-6.986	1.00	0.00
ATOM 3458 1HB ASN A 731	6.978	5.682	-4.697	1.00	0.00
ATOM 3459 2HB ASN A 731	5.406	6.307	-5.236	1.00	0.00
ATOM 3460 1HD2 ASN A 731	8.909	6.788	-7.148	1.00	0.00
ATOM 3461 2HD2 ASN A 731	8.358	5.513	-6.126	1.00	0.00
ATOM 3462 N LEU A 732	4.389	3.608	-5.654	1.00	0.00
ATOM 3463 CA LEU A 732	3.673	2.603	-4.884	1.00	0.00
ATOM 3464 C LEU A 732	3.997	1.198	-5.395	1.00	0.00
ATOM 3465 O LEU A 732	4.352	0.318	-4.621	1.00	0.00
ATOM 3466 CB LEU A 732	2.167	2.913	-4.937	1.00	0.00
ATOM 3467 CG LEU A 732	1.276	2.084	-4.002	1.00	0.00
ATOM 3468 CD1 LEU A 732	-0.051	2.820	-3.762	1.00	0.00
ATOM 3469 CD2 LEU A 732	1.004	0.675	-4.542	1.00	0.00
ATOM 3470 HN LEU A 732	3.877	4.336	-6.105	1.00	0.00
ATOM 3471 HA LEU A 732	4.037	2.690	-3.860	1.00	0.00
ATOM 3472 1HB LEU A 732	1.790	2.817	-5.951	1.00	0.00
ATOM 3473 2HB LEU A 732	2.044	3.962	-4.666	1.00	0.00
ATOM 3474 HG LEU A 732	1.791	1.986	-3.050	1.00	0.00
ATOM 3475 1HD1 LEU A 732	-0.731	2.224	-3.158	1.00	0.00
ATOM 3476 2HD1 LEU A 732	-0.557	3.042	-4.701	1.00	0.00
ATOM 3477 3HD1 LEU A 732	0.112	3.764	-3.240	1.00	0.00
ATOM 3478 1HD2 LEU A 732	0.728	0.714	-5.592	1.00	0.00



87/208

ATOM	3479	2HD2 LEU A 732	0.188	0.202	-3.998	1.00	0.00
ATOM	3480	3HD2 LEU A 732	1.865	0.018	-4.444	1.00	0.00
ATOM	3481	N LEU A 733	3.882	1.025	-6.730	1.00	0.00
ATOM	3482	CA LEU A 733	4.123	-0.307	-7.268	1.00	0.00
ATOM	3483	C LEU A 733	5.569	-0.716	-7.057	1.00	0.00
ATOM	3484	O LEU A 733	5.843	-1.876	-6.783	1.00	0.00
ATOM	3485	CB LEU A 733	3.761	-0.454	-8.753	1.00	0.00
ATOM	3486	CG LEU A 733	2.286	-0.825	-8.982	1.00	0.00
ATOM	3487	CD1 LEU A 733	1.429	0.428	-9.126	1.00	0.00
ATOM	3488	CD2 LEU A 733	2.141	-1.718	-10.214	1.00	0.00
ATOM	3489	HN LEU A 733	3.603	1.798	-7.310	1.00	0.00
ATOM	3490	HA LEU A 733	3.518	-0.998	-6.677	1.00	0.00
ATOM	3491	1HB LEU A 733	4.363	-1.258	-9.182	1.00	0.00
ATOM	3492	2HB LEU A 733	4.043	0.440	-9.313	1.00	0.00
ATOM	3493	HG LEU A 733	1.916	-1.402	-8.133	1.00	0.00
ATOM	3494	1HD1 LEU A 733	1.798	1.058	-9.937	1.00	0.00
ATOM	3495	2HD1 LEU A 733	1.450	1.008	-8.204	1.00	0.00
ATOM	3496	3HD1 LEU A 733	0.392	0.179	-9.350	1.00	0.00
ATOM	3497	1HD2 LEU A 733	2.708	-2.644	-10.104	1.00	0.00
ATOM	3498	2HD2 LEU A 733	2.518	-1.194	-11.090	1.00	0.00
ATOM	3499	3HD2 LEU A 733	1.101	-1.995	-10.389	1.00	0.00
ATOM	3500	N ASN A 734	6.483	0.268	-7.192	1.00	0.00
ATOM	3501	CA ASN A 734	7.872	-0.044	-7.046	1.00	0.00
ATOM	3502	C ASN A 734	8.076	-0.607	-5.680	1.00	0.00
ATOM	3503	O ASN A 734	8.776	-1.603	-5.507	1.00	0.00
ATOM	3504	CB ASN A 734	8.785	1.188	-7.172	1.00	0.00
ATOM	3505	CG ASN A 734	8.736	1.676	-8.611	1.00	0.00
ATOM	3506	OD1 ASN A 734	8.794	0.888	-9.554	1.00	0.00
ATOM	3507	ND2 ASN A 734	8.622	3.020	-8.790	1.00	0.00
ATOM	3508	HN ASN A 734	6.201	1.201	-7.415	1.00	0.00
ATOM	3509	HA ASN A 734	8.111	-0.767	-7.826	1.00	0.00
ATOM	3510	1HB ASN A 734	9.812	0.928	-6.916	1.00	0.00
ATOM	3511	2HB ASN A 734	8.444	1.984	-6.511	1.00	0.00
ATOM	3512	1HD2 ASN A 734	8.576	3.623	-7.994	1.00	0.00
ATOM	3513	2HD2 ASN A 734	8.584	3.419	-9.706	1.00	0.00
ATOM	3514	N TYR A 735	7.472	0.061	-4.663	1.00	0.00
ATOM	3515	CA TYR A 735	7.712	-0.419	-3.297	1.00	0.00
ATOM	3516	C TYR A 735	6.993	-1.750	-3.052	1.00	0.00
ATOM	3517	O TYR A 735	7.519	-2.627	-2.381	1.00	0.00
ATOM	3518	CB TYR A 735	7.350	0.616	-2.209	1.00	0.00
ATOM	3519	CG TYR A 735	7.674	0.144	-0.800	1.00	0.00
ATOM	3520	CD1 TYR A 735	8.850	-0.555	-0.517	1.00	0.00
ATOM	3521	CD2 TYR A 735	6.788	0.380	0.250	1.00	0.00
ATOM	3522	CE1 TYR A 735	9.119	-1.018	0.764	1.00	0.00
ATOM	3523	CE2 TYR A 735	7.061	-0.082	1.536	1.00	0.00
ATOM	3524	CZ TYR A 735	8.232	-0.775	1.800	1.00	0.00
ATOM	3525	OH TYR A 735	8.521	-1.222	3.077	1.00	0.00
ATOM	3526	HN TYR A 735	6.917	0.875	-4.864	1.00	0.00
ATOM	3527	HA TYR A 735	8.784	-0.616	-3.250	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

88/208

ATOM	3528	IHB	TYR	A	735	6.287	0.852	-2.275	1.00	0.00
ATOM	3529	2HB	TYR	A	735	7.886	1.547	-2.393	1.00	0.00
ATOM	3530	HD1	TYR	A	735	9.577	-0.763	-1.285	1.00	0.00
ATOM	3531	HE1	TYR	A	735	10.023	-1.577	0.952	1.00	0.00
ATOM	3532	HD2	TYR	A	735	5.867	0.913	0.069	1.00	0.00
ATOM	3533	HE2	TYR	A	735	6.349	0.077	2.330	1.00	0.00
ATOM	3534	HH	TYR	A	735	9.007	-0.572	3.589	1.00	0.00
ATOM	3535	N	CYS	A	736	5.797	-1.868	-3.656	1.00	0.00
ATOM	3536	CA	CYS	A	736	5.021	-3.096	-3.545	1.00	0.00
ATOM	3537	C	CYS	A	736	5.847	-4.286	-4.026	1.00	0.00
ATOM	3538	O	CYS	A	736	5.925	-5.320	-3.369	1.00	0.00
ATOM	3539	CB	CYS	A	736	3.696	-2.947	-4.303	1.00	0.00
ATOM	3540	SG	CYS	A	736	2.461	-4.186	-3.834	1.00	0.00
ATOM	3541	HN	CYS	A	736	5.452	-1.090	-4.182	1.00	0.00
ATOM	3542	HA	CYS	A	736	4.829	-3.258	-2.490	1.00	0.00
ATOM	3543	IHB	CYS	A	736	3.856	-2.988	-5.382	1.00	0.00
ATOM	3544	2HB	CYS	A	736	3.270	-1.966	-4.093	1.00	0.00
ATOM	3545	HG	CYS	A	736	1.304	-3.914	-4.440	1.00	0.00
ATOM	3546	N	PHE	A	737	6.506	-4.064	-5.183	1.00	0.00
ATOM	3547	CA	PHE	A	737	7.249	-5.179	-5.733	1.00	0.00
ATOM	3548	C	PHE	A	737	8.514	-5.457	-4.926	1.00	0.00
ATOM	3549	O	PHE	A	737	8.950	-6.593	-4.862	1.00	0.00
ATOM	3550	CB	PHE	A	737	7.421	-5.145	-7.268	1.00	0.00
ATOM	3551	CG	PHE	A	737	8.665	-4.481	-7.801	1.00	0.00
ATOM	3552	CD1	PHE	A	737	8.577	-3.263	-8.460	1.00	0.00
ATOM	3553	CD2	PHE	A	737	9.914	-5.087	-7.676	1.00	0.00
ATOM	3554	CE1	PHE	A	737	9.711	-2.651	-8.980	1.00	0.00
ATOM	3555	CE2	PHE	A	737	11.052	-4.479	-8.191	1.00	0.00
ATOM	3556	CZ	PHE	A	737	10.951	-3.258	-8.843	1.00	0.00
ATOM	3557	HN	PHE	A	737	6.446	-3.190	-5.666	1.00	0.00
ATOM	3558	HA	PHE	A	737	6.610	-6.051	-5.573	1.00	0.00
ATOM	3559	IHB	PHE	A	737	6.537	-4.699	-7.727	1.00	0.00
ATOM	3560	2HB	PHE	A	737	7.444	-6.174	-7.632	1.00	0.00
ATOM	3561	HD1	PHE	A	737	7.613	-2.789	-8.574	1.00	0.00
ATOM	3562	HD2	PHE	A	737	10.007	-6.045	-7.184	1.00	0.00
ATOM	3563	HE1	PHE	A	737	9.625	-1.701	-9.490	1.00	0.00
ATOM	3564	HE2	PHE	A	737	12.014	-4.959	-8.085	1.00	0.00
ATOM	3565	HZ	PHE	A	737	11.833	-2.781	-9.246	1.00	0.00
ATOM	3566	N	GLN	A	738	9.120	-4.415	-4.322	1.00	0.00
ATOM	3567	CA	GLN	A	738	10.282	-4.659	-3.514	1.00	0.00
ATOM	3568	C	GLN	A	738	9.894	-5.407	-2.272	1.00	0.00
ATOM	3569	O	GLN	A	738	10.561	-6.363	-1.882	1.00	0.00
ATOM	3570	CB	GLN	A	738	11.000	-3.359	-3.105	1.00	0.00
ATOM	3571	CG	GLN	A	738	12.352	-3.577	-2.418	1.00	0.00
ATOM	3572	CD	GLN	A	738	12.102	-3.957	-0.966	1.00	0.00
ATOM	3573	OE1	GLN	A	738	11.251	-3.369	-0.301	1.00	0.00
ATOM	3574	NE2	GLN	A	738	12.856	-4.970	-0.462	1.00	0.00
ATOM	3575	HN	GLN	A	738	8.801	-3.479	-4.470	1.00	0.00
ATOM	3576	HA	GLN	A	738	10.949	-5.287	-4.104	1.00	0.00

89/208

ATOM	3577	1HB	GLN A 738	10.353	-2.805	-2.427	1.00	0.00
ATOM	3578	2HB	GLN A 738	11.159	-2.756	-3.998	1.00	0.00
ATOM	3579	1HG	GLN A 738	12.948	-2.665	-2.452	1.00	0.00
ATOM	3580	2HG	GLN A 738	12.903	-4.381	-2.908	1.00	0.00
ATOM	3581	1HE2	GLN A 738	13.630	-5.321	-0.989	1.00	0.00
ATOM	3582	2HE2	GLN A 738	12.652	-5.374	0.429	1.00	0.00
ATOM	3583	N	THR A 739	8.777	-4.983	-1.675	1.00	0.00
ATOM	3584	CA	THR A 739	8.229	-5.599	-0.472	1.00	0.00
ATOM	3585	C	THR A 739	7.769	-7.048	-0.725	1.00	0.00
ATOM	3586	O	THR A 739	7.590	-7.863	0.163	1.00	0.00
ATOM	3587	CB	THR A 739	7.024	-4.732	-0.074	1.00	0.00
ATOM	3588	OG1	THR A 739	7.468	-3.420	0.223	1.00	0.00
ATOM	3589	CG2	THR A 739	6.312	-5.263	1.159	1.00	0.00
ATOM	3590	HN	THR A 739	8.305	-4.212	-2.093	1.00	0.00
ATOM	3591	HA	THR A 739	9.007	-5.592	0.292	1.00	0.00
ATOM	3592	HB	THR A 739	6.279	-4.716	-0.884	1.00	0.00
ATOM	3593	HG1	THR A 739	7.587	-2.915	-0.587	1.00	0.00
ATOM	3594	1HG2	THR A 739	6.996	-5.820	1.792	1.00	0.00
ATOM	3595	2HG2	THR A 739	5.517	-5.941	0.871	1.00	0.00
ATOM	3596	3HG2	THR A 739	5.874	-4.459	1.746	1.00	0.00
ATOM	3597	N	PHE A 740	7.539	-7.292	-2.006	1.00	0.00
ATOM	3598	CA	PHE A 740	7.217	-8.590	-2.519	1.00	0.00
ATOM	3599	C	PHE A 740	8.461	-9.389	-2.770	1.00	0.00
ATOM	3600	O	PHE A 740	8.539	-10.564	-2.415	1.00	0.00
ATOM	3601	CB	PHE A 740	6.466	-8.465	-3.856	1.00	0.00
ATOM	3602	CG	PHE A 740	6.007	-9.806	-4.302	1.00	0.00
ATOM	3603	CD1	PHE A 740	6.865	-10.669	-4.944	1.00	0.00
ATOM	3604	CD2	PHE A 740	4.676	-10.138	-4.199	1.00	0.00
ATOM	3605	CE1	PHE A 740	6.402	-11.859	-5.454	1.00	0.00
ATOM	3606	CE2	PHE A 740	4.207	-11.323	-4.709	1.00	0.00
ATOM	3607	CZ	PHE A 740	5.072	-12.183	-5.342	1.00	0.00
ATOM	3608	HN	PHE A 740	7.342	-6.493	-2.574	1.00	0.00
ATOM	3609	HA	PHE A 740	6.596	-9.089	-1.774	1.00	0.00
ATOM	3610	1HB	PHE A 740	7.124	-8.042	-4.615	1.00	0.00
ATOM	3611	2HB	PHE A 740	5.601	-7.813	-3.738	1.00	0.00
ATOM	3612	HD1	PHE A 740	7.908	-10.410	-5.047	1.00	0.00
ATOM	3613	HD2	PHE A 740	3.992	-9.458	-3.712	1.00	0.00
ATOM	3614	HE1	PHE A 740	7.085	-12.539	-5.941	1.00	0.00
ATOM	3615	HE2	PHE A 740	3.163	-11.580	-4.612	1.00	0.00
ATOM	3616	HZ	PHE A 740	4.706	-13.112	-5.753	1.00	0.00
ATOM	3617	N	LEU A 741	9.481	-8.749	-3.373	1.00	0.00
ATOM	3618	CA	LEU A 741	10.675	-9.435	-3.772	1.00	0.00
ATOM	3619	C	LEU A 741	11.407	-10.008	-2.617	1.00	0.00
ATOM	3620	O	LEU A 741	11.870	-11.146	-2.694	1.00	0.00
ATOM	3621	CB	LEU A 741	11.668	-8.553	-4.549	1.00	0.00
ATOM	3622	CG	LEU A 741	12.941	-9.319	-4.958	1.00	0.00
ATOM	3623	CD1	LEU A 741	12.608	-10.522	-5.851	1.00	0.00
ATOM	3624	CD2	LEU A 741	13.977	-8.382	-5.600	1.00	0.00
ATOM	3625	HN	LEU A 741	9.403	-7.768	-3.547	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

90/208

ATOM	3626	HA	LEU A 741	10.356	-10.270	-4.395	1.00	0.00
ATOM	3627	IHB	LEU A 741	11.950	-7.704	-3.927	1.00	0.00
ATOM	3628	2HB	LEU A 741	11.179	-8.174	-5.445	1.00	0.00
ATOM	3629	HG	LEU A 741	13.455	-9.667	-4.062	1.00	0.00
ATOM	3630	1HD1	LEU A 741	11.955	-10.224	-6.671	1.00	0.00
ATOM	3631	2HD1	LEU A 741	12.094	-11.290	-5.273	1.00	0.00
ATOM	3632	3HD1	LEU A 741	13.521	-10.937	-6.280	1.00	0.00
ATOM	3633	1HD2	LEU A 741	14.269	-7.596	-4.904	1.00	0.00
ATOM	3634	2HD2	LEU A 741	13.557	-7.908	-6.487	1.00	0.00
ATOM	3635	3HD2	LEU A 741	14.872	-8.941	-5.873	1.00	0.00
ATOM	3636	N	ASP A 742	11.534	-9.248	-1.511	1.00	0.00
ATOM	3637	CA	ASP A 742	12.265	-9.803	-0.414	1.00	0.00
ATOM	3638	C	ASP A 742	11.571	-11.053	0.018	1.00	0.00
ATOM	3639	O	ASP A 742	10.347	-11.162	-0.050	1.00	0.00
ATOM	3640	CB	ASP A 742	12.541	-8.820	0.746	1.00	0.00
ATOM	3641	CG	ASP A 742	11.249	-8.276	1.322	1.00	0.00
ATOM	3642	OD1	ASP A 742	10.245	-9.033	1.325	1.00	0.00
ATOM	3643	OD2	ASP A 742	11.246	-7.093	1.757	1.00	0.00
ATOM	3644	HN	ASP A 742	11.134	-8.333	-1.460	1.00	0.00
ATOM	3645	HA	ASP A 742	13.209	-10.156	-0.828	1.00	0.00
ATOM	3646	IHB	ASP A 742	13.139	-7.982	0.386	1.00	0.00
ATOM	3647	2HB	ASP A 742	13.086	-9.330	1.540	1.00	0.00
ATOM	3648	N	LYS A 743	12.368	-12.049	0.448	1.00	0.00
ATOM	3649	CA	LYS A 743	11.832	-13.346	0.724	1.00	0.00
ATOM	3650	C	LYS A 743	10.692	-13.275	1.663	1.00	0.00
ATOM	3651	O	LYS A 743	9.628	-13.837	1.400	1.00	0.00
ATOM	3652	CB	LYS A 743	12.806	-14.309	1.412	1.00	0.00
ATOM	3653	CG	LYS A 743	12.044	-15.542	1.902	1.00	0.00
ATOM	3654	CD	LYS A 743	12.883	-16.607	2.605	1.00	0.00
ATOM	3655	CE	LYS A 743	12.022	-17.662	3.304	1.00	0.00
ATOM	3656	NZ	LYS A 743	11.056	-16.998	4.210	1.00	0.00
ATOM	3657	HN	LYS A 743	13.345	-11.880	0.575	1.00	0.00
ATOM	3658	HA	LYS A 743	11.525	-13.758	-0.236	1.00	0.00
ATOM	3659	IHB	LYS A 743	13.284	-13.811	2.255	1.00	0.00
ATOM	3660	2HB	LYS A 743	13.583	-14.611	0.709	1.00	0.00
ATOM	3661	1HG	LYS A 743	11.560	-16.005	1.044	1.00	0.00
ATOM	3662	2HG	LYS A 743	11.272	-15.210	2.594	1.00	0.00
ATOM	3663	1HD	LYS A 743	13.523	-16.124	3.344	1.00	0.00
ATOM	3664	2HD	LYS A 743	13.520	-17.098	1.870	1.00	0.00
ATOM	3665	1HE	LYS A 743	12.645	-18.329	3.899	1.00	0.00
ATOM	3666	2HE	LYS A 743	11.460	-18.241	2.571	1.00	0.00
ATOM	3667	1HZ	LYS A 743	10.178	-16.794	3.691	1.00	0.00
ATOM	3668	2HZ	LYS A 743	11.465	-16.109	4.561	1.00	0.00
ATOM	3669	3HZ	LYS A 743	10.847	-17.625	5.013	1.00	0.00
ATOM	3670	N	THR A 744	10.866	-12.578	2.792	1.00	0.00
ATOM	3671	CA	THR A 744	9.773	-12.650	3.697	1.00	0.00
ATOM	3672	C	THR A 744	9.253	-11.262	3.862	1.00	0.00
ATOM	3673	O	THR A 744	9.960	-10.390	4.369	1.00	0.00
ATOM	3674	CB	THR A 744	10.206	-13.141	5.048	1.00	0.00

91/208

ATOM 3675	OG1 THR A 744	11.103	-14.232	4.899	1.00	0.00
ATOM 3676	CG2 THR A 744	8.960	-13.680	5.773	1.00	0.00
ATOM 3677	HN THR A 744	11.693	-12.052	2.981	1.00	0.00
ATOM 3678	HA THR A 744	9.043	-13.332	3.261	1.00	0.00
ATOM 3679	HB THR A 744	10.718	-12.349	5.594	1.00	0.00
ATOM 3680	HG1 THR A 744	11.846	-13.909	4.407	1.00	0.00
ATOM 3681	1HG2 THR A 744	8.820	-14.740	5.563	1.00	0.00
ATOM 3682	2HG2 THR A 744	8.069	-13.150	5.436	1.00	0.00
ATOM 3683	3HG2 THR A 744	9.071	-13.562	6.851	1.00	0.00
ATOM 3684	N MET A 745	8.018	-10.964	3.408	1.00	0.00
ATOM 3685	CA MET A 745	7.428	-9.642	3.726	1.00	0.00
ATOM 3686	C MET A 745	5.989	-9.601	3.232	1.00	0.00
ATOM 3687	O MET A 745	5.055	-9.884	3.973	1.00	0.00
ATOM 3688	CB MET A 745	8.233	-8.382	3.310	1.00	0.00
ATOM 3689	CG MET A 745	7.813	-7.093	4.023	1.00	0.00
ATOM 3690	SD MET A 745	9.021	-5.787	3.661	1.00	0.00
ATOM 3691	CE MET A 745	7.992	-4.302	3.617	1.00	0.00
ATOM 3692	HN MET A 745	7.516	-11.616	2.840	1.00	0.00
ATOM 3693	HA MET A 745	7.362	-9.591	4.801	1.00	0.00
ATOM 3694	1HB MET A 745	8.199	-8.227	2.245	1.00	0.00
ATOM 3695	2HB MET A 745	9.288	-8.489	3.533	1.00	0.00
ATOM 3696	1HG MET A 745	7.795	-7.286	5.094	1.00	0.00
ATOM 3697	2HG MET A 745	6.810	-6.798	3.719	1.00	0.00
ATOM 3698	1HE MET A 745	8.417	-3.530	4.257	1.00	0.00
ATOM 3699	2HE MET A 745	6.972	-4.501	3.945	1.00	0.00
ATOM 3700	3HE MET A 745	7.986	-3.875	2.615	1.00	0.00
ATOM 3701	N SER A 746	5.851	-9.230	1.946	1.00	0.00
ATOM 3702	CA SER A 746	4.516	-9.190	1.377	1.00	0.00
ATOM 3703	C SER A 746	4.071	-10.623	1.276	1.00	0.00
ATOM 3704	O SER A 746	4.874	-11.495	0.961	1.00	0.00
ATOM 3705	CB SER A 746	4.501	-8.593	-0.037	1.00	0.00
ATOM 3706	OG SER A 746	3.188	-8.162	-0.377	1.00	0.00
ATOM 3707	HN SER A 746	6.665	-9.030	1.391	1.00	0.00
ATOM 3708	HA SER A 746	3.877	-8.626	2.057	1.00	0.00
ATOM 3709	1HB SER A 746	4.846	-9.345	-0.755	1.00	0.00
ATOM 3710	2HB SER A 746	5.187	-7.749	-0.090	1.00	0.00
ATOM 3711	HG SER A 746	3.159	-7.827	-1.275	1.00	0.00
ATOM 3712	N ILE A 747	2.778	-10.859	1.568	1.00	0.00
ATOM 3713	CA ILE A 747	2.333	-12.194	1.377	1.00	0.00
ATOM 3714	C ILE A 747	2.368	-12.310	-0.104	1.00	0.00
ATOM 3715	O ILE A 747	1.618	-11.654	-0.825	1.00	0.00
ATOM 3716	CB ILE A 747	0.939	-12.479	1.863	1.00	0.00
ATOM 3717	CG1 ILE A 747	0.778	-12.082	3.341	1.00	0.00
ATOM 3718	CG2 ILE A 747	0.700	-13.986	1.658	1.00	0.00
ATOM 3719	CD1 ILE A 747	0.813	-10.575	3.581	1.00	0.00
ATOM 3720	HN ILE A 747	2.179	-10.147	1.933	1.00	0.00
ATOM 3721	HA ILE A 747	3.042	-12.826	1.911	1.00	0.00
ATOM 3722	HB ILE A 747	0.211	-11.897	1.297	1.00	0.00
ATOM 3723	1HG2 ILE A 747	1.303	-14.570	2.353	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

92/208

ATOM	3724	2HG2	ILE A 747	0.978	-14.277	0.645	1.00	0.00
ATOM	3725	3HG2	ILE A 747	-0.348	-14.228	1.835	1.00	0.00
ATOM	3726	1HG1	ILE A 747	1.579	-12.545	3.916	1.00	0.00
ATOM	3727	2HG1	ILE A 747	-0.173	-12.471	3.704	1.00	0.00
ATOM	3728	1HD1	ILE A 747	0.129	-10.061	2.906	1.00	0.00
ATOM	3729	2HD1	ILE A 747	1.816	-10.189	3.403	1.00	0.00
ATOM	3730	3HD1	ILE A 747	0.510	-10.350	4.604	1.00	0.00
ATOM	3731	N	GLU A 748	3.284	-13.156	-0.596	1.00	0.00
ATOM	3732	CA	GLU A 748	3.436	-13.371	-2.000	1.00	0.00
ATOM	3733	C	GLU A 748	2.141	-13.951	-2.449	1.00	0.00
ATOM	3734	O	GLU A 748	1.764	-13.859	-3.616	1.00	0.00
ATOM	3735	CB	GLU A 748	4.568	-14.372	-2.304	1.00	0.00
ATOM	3736	CG	GLU A 748	4.775	-14.670	-3.789	1.00	0.00
ATOM	3737	CD	GLU A 748	3.903	-15.864	-4.150	1.00	0.00
ATOM	3738	OE1	GLU A 748	3.323	-16.474	-3.212	1.00	0.00
ATOM	3739	OE2	GLU A 748	3.813	-16.188	-5.363	1.00	0.00
ATOM	3740	HN	GLU A 748	3.877	-13.651	0.039	1.00	0.00
ATOM	3741	HA	GLU A 748	3.656	-12.402	-2.448	1.00	0.00
ATOM	3742	1HB	GLU A 748	4.346	-15.308	-1.793	1.00	0.00
ATOM	3743	2HB	GLU A 748	5.497	-13.973	-1.900	1.00	0.00
ATOM	3744	1HG	GLU A 748	5.819	-14.911	-3.990	1.00	0.00
ATOM	3745	2HG	GLU A 748	4.484	-13.813	-4.397	1.00	0.00
ATOM	3746	N	PHE A 749	1.432	-14.561	-1.486	1.00	0.00
ATOM	3747	CA	PHE A 749	0.228	-15.295	-1.685	1.00	0.00
ATOM	3748	C	PHE A 749	-1.022	-14.586	-2.108	1.00	0.00
ATOM	3749	O	PHE A 749	-1.822	-15.245	-2.771	1.00	0.00
ATOM	3750	CB	PHE A 749	-0.049	-16.229	-0.502	1.00	0.00
ATOM	3751	CG	PHE A 749	1.105	-17.172	-0.580	1.00	0.00
ATOM	3752	CD1	PHE A 749	1.105	-18.179	-1.517	1.00	0.00
ATOM	3753	CD2	PHE A 749	2.252	-16.944	0.145	1.00	0.00
ATOM	3754	CE1	PHE A 749	2.221	-18.959	-1.716	1.00	0.00
ATOM	3755	CE2	PHE A 749	3.369	-17.725	-0.043	1.00	0.00
ATOM	3756	CZ	PHE A 749	3.358	-18.730	-0.980	1.00	0.00
ATOM	3757	HN	PHE A 749	1.779	-14.494	-0.552	1.00	0.00
ATOM	3758	HA	PHE A 749	0.350	-15.868	-2.604	1.00	0.00
ATOM	3759	1HB	PHE A 749	-0.995	-16.757	-0.614	1.00	0.00
ATOM	3760	2HB	PHE A 749	-0.054	-15.693	0.447	1.00	0.00
ATOM	3761	HD1	PHE A 749	0.216	-18.361	-2.104	1.00	0.00
ATOM	3762	HD2	PHE A 749	2.276	-16.143	0.869	1.00	0.00
ATOM	3763	HE1	PHE A 749	2.203	-19.750	-2.450	1.00	0.00
ATOM	3764	HE2	PHE A 749	4.256	-17.548	0.547	1.00	0.00
ATOM	3765	HZ	PHE A 749	4.237	-19.337	-1.137	1.00	0.00
ATOM	3766	N	PRO A 750	-1.315	-13.342	-1.805	1.00	0.00
ATOM	3767	CA	PRO A 750	-2.560	-12.833	-2.313	1.00	0.00
ATOM	3768	C	PRO A 750	-2.536	-12.817	-3.807	1.00	0.00
ATOM	3769	O	PRO A 750	-1.746	-12.081	-4.395	1.00	0.00
ATOM	3770	CB	PRO A 750	-2.791	-11.502	-1.606	1.00	0.00
ATOM	3771	CG	PRO A 750	-2.100	-11.720	-0.244	1.00	0.00
ATOM	3772	CD	PRO A 750	-0.975	-12.738	-0.529	1.00	0.00

93/208

ATOM 3773 1HD PRO A 750	-0.006	-12.243	-0.593	1.00	0.00
ATOM 3774 2HD PRO A 750	-0.931	-13.501	0.248	1.00	0.00
ATOM 3775 HA PRO A 750	-3.366	-13.534	-2.096	1.00	0.00
ATOM 3776 1HB PRO A 750	-3.854	-11.293	-1.486	1.00	0.00
ATOM 3777 2HB PRO A 750	-2.341	-10.675	-2.155	1.00	0.00
ATOM 3778 1HG PRO A 750	-1.692	-10.785	0.139	1.00	0.00
ATOM 3779 2HG PRO A 750	-2.803	-12.112	0.491	1.00	0.00
ATOM 3780 N GLU A 751	-3.415	-13.633	-4.421	1.00	0.00
ATOM 3781 CA GLU A 751	-3.460	-13.836	-5.840	1.00	0.00
ATOM 3782 C GLU A 751	-3.919	-12.660	-6.642	1.00	0.00
ATOM 3783 O GLU A 751	-3.277	-12.291	-7.623	1.00	0.00
ATOM 3784 CB GLU A 751	-4.349	-15.034	-6.212	1.00	0.00
ATOM 3785 CG GLU A 751	-5.788	-14.904	-5.711	1.00	0.00
ATOM 3786 CD GLU A 751	-6.544	-16.157	-6.130	1.00	0.00
ATOM 3787 OE1 GLU A 751	-6.025	-17.274	-5.868	1.00	0.00
ATOM 3788 OE2 GLU A 751	-7.649	-16.014	-6.717	1.00	0.00
ATOM 3789 HN GLU A 751	-4.073	-14.126	-3.853	1.00	0.00
ATOM 3790 HA GLU A 751	-2.436	-14.006	-6.171	1.00	0.00
ATOM 3791 1HB GLU A 751	-3.912	-15.937	-5.789	1.00	0.00
ATOM 3792 2HB GLU A 751	-4.364	-15.135	-7.296	1.00	0.00
ATOM 3793 1HG GLU A 751	-6.269	-14.030	-6.150	1.00	0.00
ATOM 3794 2HG GLU A 751	-5.810	-14.815	-4.625	1.00	0.00
ATOM 3795 N MET A 752	-5.033	-12.022	-6.240	1.00	0.00
ATOM 3796 CA MET A 752	-5.558	-10.951	-7.036	1.00	0.00
ATOM 3797 C MET A 752	-4.576	-9.828	-7.065	1.00	0.00
ATOM 3798 O MET A 752	-4.358	-9.205	-8.103	1.00	0.00
ATOM 3799 CB MET A 752	-6.887	-10.401	-6.498	1.00	0.00
ATOM 3800 CG MET A 752	-7.528	-9.365	-7.423	1.00	0.00
ATOM 3801 SD MET A 752	-8.234	-10.030	-8.960	1.00	0.00
ATOM 3802 CE MET A 752	-8.804	-8.414	-9.560	1.00	0.00
ATOM 3803 HN MET A 752	-5.491	-12.294	-5.393	1.00	0.00
ATOM 3804 HA MET A 752	-5.697	-11.348	-8.041	1.00	0.00
ATOM 3805 1HB MET A 752	-6.710	-9.942	-5.526	1.00	0.00
ATOM 3806 2HB MET A 752	-7.582	-11.229	-6.364	1.00	0.00
ATOM 3807 1HG MET A 752	-6.772	-8.630	-7.698	1.00	0.00
ATOM 3808 2HG MET A 752	-8.329	-8.863	-6.881	1.00	0.00
ATOM 3809 1HE MET A 752	-7.986	-7.695	-9.501	1.00	0.00
ATOM 3810 2HE MET A 752	-9.627	-8.057	-8.941	1.00	0.00
ATOM 3811 3HE MET A 752	-9.121	-8.495	-10.600	1.00	0.00
ATOM 3812 N LEU A 753	-3.980	-9.571	-5.881	1.00	0.00
ATOM 3813 CA LEU A 753	-3.011	-8.486	-5.797	1.00	0.00
ATOM 3814 C LEU A 753	-1.796	-8.816	-6.679	1.00	0.00
ATOM 3815 O LEU A 753	-1.275	-8.016	-7.411	1.00	0.00
ATOM 3816 CB LEU A 753	-2.612	-8.246	-4.332	1.00	0.00
ATOM 3817 CG LEU A 753	-1.716	-7.009	-4.115	1.00	0.00
ATOM 3818 CD1 LEU A 753	-2.411	-5.703	-4.529	1.00	0.00
ATOM 3819 CD2 LEU A 753	-1.262	-6.929	-2.652	1.00	0.00
ATOM 3820 HN LEU A 753	-4.193	-10.142	-5.091	1.00	0.00
ATOM 3821 HA LEU A 753	-3.510	-7.604	-6.201	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

94/208

ATOM	3822	1HB	LEU A 753	-2.102	-9.133	-3.950	1.00	0.00
ATOM	3823	2HB	LEU A 753	-3.513	-8.138	-3.727	1.00	0.00
ATOM	3824	HG	LEU A 753	-0.817	-7.118	-4.725	1.00	0.00
ATOM	3825	1HD1	LEU A 753	-2.614	-5.679	-5.599	1.00	0.00
ATOM	3826	2HD1	LEU A 753	-1.782	-4.841	-4.304	1.00	0.00
ATOM	3827	3HD1	LEU A 753	-3.356	-5.572	-4.002	1.00	0.00
ATOM	3828	1HD2	LEU A 753	-2.112	-6.817	-1.977	1.00	0.00
ATOM	3829	2HD2	LEU A 753	-0.590	-6.087	-2.490	1.00	0.00
ATOM	3830	3HD2	LEU A 753	-0.728	-7.835	-2.364	1.00	0.00
ATOM	3831	N	ALA A 754	-1.355	-10.050	-6.651	1.00	0.00
ATOM	3832	CA	ALA A 754	-0.204	-10.417	-7.422	1.00	0.00
ATOM	3833	C	ALA A 754	-0.537	-10.216	-8.862	1.00	0.00
ATOM	3834	O	ALA A 754	0.294	-9.759	-9.649	1.00	0.00
ATOM	3835	CB	ALA A 754	0.178	-11.896	-7.250	1.00	0.00
ATOM	3836	HN	ALA A 754	-1.817	-10.738	-6.092	1.00	0.00
ATOM	3837	HA	ALA A 754	0.613	-9.777	-7.089	1.00	0.00
ATOM	3838	1HB	ALA A 754	-0.640	-12.544	-7.564	1.00	0.00
ATOM	3839	2HB	ALA A 754	0.394	-12.110	-6.203	1.00	0.00
ATOM	3840	3HB	ALA A 754	1.050	-12.133	-7.859	1.00	0.00
ATOM	3841	N	GLU A 755	-1.786	-10.545	-9.230	1.00	0.00
ATOM	3842	CA	GLU A 755	-2.225	-10.455	-10.588	1.00	0.00
ATOM	3843	C	GLU A 755	-2.065	-9.055	-11.070	1.00	0.00
ATOM	3844	O	GLU A 755	-1.477	-8.828	-12.127	1.00	0.00
ATOM	3845	CB	GLU A 755	-3.715	-10.810	-10.727	1.00	0.00
ATOM	3846	CG	GLU A 755	-4.273	-10.739	-12.149	1.00	0.00
ATOM	3847	CD	GLU A 755	-5.752	-11.092	-12.056	1.00	0.00
ATOM	3848	OE1	GLU A 755	-6.066	-12.306	-11.925	1.00	0.00
ATOM	3849	OE2	GLU A 755	-6.587	-10.150	-12.100	1.00	0.00
ATOM	3850	HN	GLU A 755	-2.427	-10.864	-8.532	1.00	0.00
ATOM	3851	HA	GLU A 755	-1.614	-11.147	-11.167	1.00	0.00
ATOM	3852	1HB	GLU A 755	-4.288	-10.128	-10.101	1.00	0.00
ATOM	3853	2HB	GLU A 755	-3.860	-11.823	-10.353	1.00	0.00
ATOM	3854	1HG	GLU A 755	-3.767	-11.451	-12.801	1.00	0.00
ATOM	3855	2HG	GLU A 755	-4.161	-9.736	-12.561	1.00	0.00
ATOM	3856	N	ILE A 756	-2.558	-8.063	-10.300	1.00	0.00
ATOM	3857	CA	ILE A 756	-2.405	-6.729	-10.798	1.00	0.00
ATOM	3858	C	ILE A 756	-0.951	-6.435	-10.893	1.00	0.00
ATOM	3859	O	ILE A 756	-0.505	-5.902	-11.910	1.00	0.00
ATOM	3860	CB	ILE A 756	-3.029	-5.638	-9.952	1.00	0.00
ATOM	3861	CG1	ILE A 756	-2.921	-4.241	-10.627	1.00	0.00
ATOM	3862	CG2	ILE A 756	-2.437	-5.706	-8.536	1.00	0.00
ATOM	3863	CD1	ILE A 756	-1.513	-3.634	-10.808	1.00	0.00
ATOM	3864	HN	ILE A 756	-3.006	-8.250	-9.427	1.00	0.00
ATOM	3865	HA	ILE A 756	-2.860	-6.726	-11.788	1.00	0.00
ATOM	3866	HB	ILE A 756	-4.110	-5.774	-9.909	1.00	0.00
ATOM	3867	1HG2	ILE A 756	-1.356	-5.563	-8.563	1.00	0.00
ATOM	3868	2HG2	ILE A 756	-2.637	-6.680	-8.090	1.00	0.00
ATOM	3869	3HG2	ILE A 756	-2.864	-4.922	-7.911	1.00	0.00
ATOM	3870	1HG1	ILE A 756	-3.504	-3.542	-10.031	1.00	0.00



95/208

ATOM 3871 2HG1 ILE A 756	-3.374	-4.317	-11.613	1.00	0.00
ATOM 3872 1HD1 ILE A 756	-1.016	-4.066	-11.676	1.00	0.00
ATOM 3873 2HD1 ILE A 756	-0.898	-3.840	-9.931	1.00	0.00
ATOM 3874 3HD1 ILE A 756	-1.584	-2.557	-10.961	1.00	0.00
ATOM 3875 N ILE A 757	-0.175	-6.762	-9.850	1.00	0.00
ATOM 3876 CA ILE A 757	1.184	-6.312	-9.796	1.00	0.00
ATOM 3877 C ILE A 757	1.931	-6.758	-11.008	1.00	0.00
ATOM 3878 O ILE A 757	2.694	-5.986	-11.586	1.00	0.00
ATOM 3879 CB ILE A 757	1.925	-6.851	-8.613	1.00	0.00
ATOM 3880 CG1 ILE A 757	1.289	-6.331	-7.315	1.00	0.00
ATOM 3881 CG2 ILE A 757	3.410	-6.491	-8.781	1.00	0.00
ATOM 3882 CD1 ILE A 757	1.268	-4.806	-7.228	1.00	0.00
ATOM 3883 HN ILE A 757	-0.547	-7.322	-9.109	1.00	0.00
ATOM 3884 HA ILE A 757	1.151	-5.224	-9.755	1.00	0.00
ATOM 3885 HB ILE A 757	1.805	-7.933	-8.555	1.00	0.00
ATOM 3886 1HG2 ILE A 757	3.519	-5.482	-9.180	1.00	0.00
ATOM 3887 2HG2 ILE A 757	3.889	-7.181	-9.475	1.00	0.00
ATOM 3888 3HG2 ILE A 757	3.917	-6.529	-7.817	1.00	0.00
ATOM 3889 1HG1 ILE A 757	1.849	-6.724	-6.468	1.00	0.00
ATOM 3890 2HG1 ILE A 757	0.267	-6.701	-7.252	1.00	0.00
ATOM 3891 1HD1 ILE A 757	0.559	-4.389	-7.943	1.00	0.00
ATOM 3892 2HD1 ILE A 757	2.254	-4.402	-7.456	1.00	0.00
ATOM 3893 3HD1 ILE A 757	0.965	-4.490	-6.230	1.00	0.00
ATOM 3894 N THR A 758	1.699	-8.009	-11.440	1.00	0.00
ATOM 3895 CA THR A 758	2.403	-8.548	-12.565	1.00	0.00
ATOM 3896 C THR A 758	2.097	-7.753	-13.792	1.00	0.00
ATOM 3897 O THR A 758	2.966	-7.545	-14.637	1.00	0.00
ATOM 3898 CB THR A 758	2.045	-9.979	-12.854	1.00	0.00
ATOM 3899 OG1 THR A 758	2.968	-10.535	-13.779	1.00	0.00
ATOM 3900 CG2 THR A 758	0.620	-10.034	-13.435	1.00	0.00
ATOM 3901 HN THR A 758	1.023	-8.573	-10.967	1.00	0.00
ATOM 3902 HA THR A 758	3.465	-8.468	-12.334	1.00	0.00
ATOM 3903 HB THR A 758	2.079	-10.570	-11.939	1.00	0.00
ATOM 3904 HG1 THR A 758	3.149	-9.862	-14.421	1.00	0.00
ATOM 3905 1HG2 THR A 758	0.650	-10.130	-14.520	1.00	0.00
ATOM 3906 2HG2 THR A 758	0.079	-9.120	-13.192	1.00	0.00
ATOM 3907 3HG2 THR A 758	0.084	-10.895	-13.035	1.00	0.00
ATOM 3908 N ASN A 759	0.852	-7.259	-13.912	1.00	0.00
ATOM 3909 CA ASN A 759	0.449	-6.558	-15.094	1.00	0.00
ATOM 3910 C ASN A 759	1.381	-5.433	-15.388	1.00	0.00
ATOM 3911 O ASN A 759	1.869	-5.304	-16.509	1.00	0.00
ATOM 3912 CB ASN A 759	-0.951	-5.941	-14.956	1.00	0.00
ATOM 3913 CG ASN A 759	-1.259	-5.187	-16.241	1.00	0.00
ATOM 3914 OD1 ASN A 759	-1.632	-4.013	-16.206	1.00	0.00
ATOM 3915 ND2 ASN A 759	-1.094	-5.868	-17.405	1.00	0.00
ATOM 3916 HN ASN A 759	0.199	-7.383	-13.165	1.00	0.00
ATOM 3917 HA ASN A 759	0.464	-7.282	-15.909	1.00	0.00
ATOM 3918 1HB ASN A 759	-0.983	-5.249	-14.115	1.00	0.00
ATOM 3919 2HB ASN A 759	-1.700	-6.719	-14.806	1.00	0.00

SUBSTITUTE SHEET (RULE 26)

96/208

ATOM	3920	1HD2 ASN A 759	-0.784	-6.819	-17.383	1.00	0.00
ATOM	3921	2HD2 ASN A 759	-1.278	-5.437	-18.288	1.00	0.00
ATOM	3922	N GLN A 760	1.663	-4.583	-14.389	1.00	0.00
ATOM	3923	CA GLN A 760	2.499	-3.460	-14.673	1.00	0.00
ATOM	3924	C GLN A 760	3.920	-3.842	-14.935	1.00	0.00
ATOM	3925	O GLN A 760	4.581	-3.218	-15.763	1.00	0.00
ATOM	3926	CB GLN A 760	2.341	-2.318	-13.653	1.00	0.00
ATOM	3927	CG GLN A 760	0.911	-1.764	-13.764	1.00	0.00
ATOM	3928	CD GLN A 760	0.769	-0.440	-13.032	1.00	0.00
ATOM	3929	OE1 GLN A 760	1.510	0.510	-13.277	1.00	0.00
ATOM	3930	NE2 GLN A 760	-0.221	-0.373	-12.102	1.00	0.00
ATOM	3931	HN GLN A 760	1.298	-4.733	-13.470	1.00	0.00
ATOM	3932	HA GLN A 760	2.225	-3.112	-15.669	1.00	0.00
ATOM	3933	1HB GLN A 760	3.065	-1.530	-13.860	1.00	0.00
ATOM	3934	2HB GLN A 760	2.521	-2.690	-12.645	1.00	0.00
ATOM	3935	1HG GLN A 760	0.207	-2.474	-13.330	1.00	0.00
ATOM	3936	2HG GLN A 760	0.659	-1.606	-14.812	1.00	0.00
ATOM	3937	1HE2 GLN A 760	-0.702	-1.206	-11.828	1.00	0.00
ATOM	3938	2HE2 GLN A 760	-0.480	0.497	-11.683	1.00	0.00
ATOM	3939	N ILE A 761	4.442	-4.879	-14.248	1.00	0.00
ATOM	3940	CA ILE A 761	5.781	-5.292	-14.553	1.00	0.00
ATOM	3941	C ILE A 761	5.742	-6.011	-15.908	1.00	0.00
ATOM	3942	1OCT ILE A 761	5.322	-5.360	-16.902	1.00	0.00
ATOM	3943	CB ILE A 761	6.385	-6.218	-13.530	1.00	0.00
ATOM	3944	CG1 ILE A 761	7.830	-6.571	-13.928	1.00	0.00
ATOM	3945	CG2 ILE A 761	5.457	-7.428	-13.332	1.00	0.00
ATOM	3946	CD1 ILE A 761	8.597	-7.355	-12.864	1.00	0.00
ATOM	3947	2OCT ILE A 761	6.129	-7.209	-15.978	1.00	0.00
ATOM	3948	HN ILE A 761	3.908	-5.347	-13.544	1.00	0.00
ATOM	3949	HA ILE A 761	6.375	-4.381	-14.624	1.00	0.00
ATOM	3950	HB ILE A 761	6.414	-5.651	-12.601	1.00	0.00
ATOM	3951	1HG2 ILE A 761	4.449	-7.102	-13.075	1.00	0.00
ATOM	3952	2HG2 ILE A 761	5.825	-8.056	-12.520	1.00	0.00
ATOM	3953	3HG2 ILE A 761	5.399	-8.013	-14.250	1.00	0.00
ATOM	3954	1HG1 ILE A 761	8.369	-5.647	-14.132	1.00	0.00
ATOM	3955	2HG1 ILE A 761	7.804	-7.162	-14.842	1.00	0.00
ATOM	3956	1HD1 ILE A 761	8.098	-8.299	-12.647	1.00	0.00
ATOM	3957	2HD1 ILE A 761	8.649	-6.781	-11.939	1.00	0.00
ATOM	3958	3HD1 ILE A 761	9.604	-7.578	-13.214	1.00	0.00
ATOM	3959	HCT ILE A 761	5.361	-4.423	-16.765	1.00	0.00
ATOM	3960	O HOH W 516	-9.097	2.914	0.913	1.00	0.00
ATOM	3961	1H HOH W 516	-8.853	3.396	0.115	1.00	0.00
ATOM	3962	2H HOH W 516	-8.335	2.330	1.052	1.00	0.00
ATOM	3963	NA+ CIP C 206	6.097	8.962	-3.974	1.00	0.00
ATOM	3964	NA+ CIP C 157	-9.340	-4.397	-27.602	1.00	0.00
ATOM	3965	NA+ CIP C 105	-8.364	-4.063	14.059	1.00	0.00
ATOM	3966	NA+ CIP C 184	-23.434	28.968	-12.650	1.00	0.00
ATOM	3967	NA+ CIP C 202	3.261	11.659	-12.120	1.00	0.00
ATOM	3968	NA+ CIP C 166	-15.650	5.434	-32.841	1.00	0.00

97/208

ATOM	3969	NA+	CIP C 234	-7.350	-13.381	-10.083	1.00	0.00
ATOM	3970	NA+	CIP C 120	9.673	4.279	-1.053	1.00	0.00
ATOM	3971	CL-	CIM C 58	-20.663	-6.966	-18.429	1.00	0.00
ATOM	3972	NA+	CIP C 167	-16.694	-0.528	-26.996	1.00	0.00
ATOM	3973	CL-	CIM C 174	-24.680	17.196	-19.047	1.00	0.00
ATOM	3974	NA+	CIP C 16	-22.819	13.330	-4.433	1.00	0.00
ATOM	3975	NA+	CIP C 227	1.631	-16.295	-6.675	1.00	0.00
ATOM	3976	NA+	CIP C 221	11.345	-4.726	2.532	1.00	0.00
ATOM	3977	CL-	CIM C 93	-13.515	6.310	6.654	1.00	0.00
ATOM	3978	CL-	CIM C 160	-10.213	-4.624	-36.213	1.00	0.00
ATOM	3979	CL-	CIM C 178	-24.595	17.570	-9.392	1.00	0.00
ATOM	3980	CL-	CIM C 55	-18.222	-8.698	-11.429	1.00	0.00
ATOM	3981	CL-	CIM C 183	-15.467	17.246	-10.379	1.00	0.00

END

98/208

Fig 13

REMARK 1 grfromer modeller, no optimisation july 15 1998

ATOM	1	N	GLN	1	1	31.226	-1.970	94.273	1.00	5.90
ATOM	2	CA	GLN	1	1	32.061	-3.185	94.135	1.00	5.90
ATOM	3	C	GLN	1	1	33.238	-2.949	93.251	1.00	5.90
ATOM	4	O	GLN	1	1	33.964	-1.969	93.402	1.00	5.90
ATOM	5	CB	GLN	1	1	31.246	-4.344	93.534	1.00	5.90
ATOM	6	CG	GLN	1	1	30.248	-4.977	94.504	1.00	5.90
ATOM	7	CD	GLN	1	1	31.030	-5.896	95.434	1.00	5.90
ATOM	8	OE1	GLN	1	1	30.460	-6.569	96.291	1.00	5.90
ATOM	9	NE2	GLN	1	1	32.378	-5.931	95.256	1.00	5.90
ATOM	10	N	LEU	1	2	33.462	-3.888	92.314	1.00	0.97
ATOM	11	CA	LEU	1	2	34.556	-3.825	91.394	1.00	0.97
ATOM	12	C	LEU	1	2	34.400	-2.709	90.407	1.00	0.97
ATOM	13	O	LEU	1	2	35.388	-2.108	89.988	1.00	0.97
ATOM	14	CB	LEU	1	2	34.752	-5.124	90.594	1.00	0.97
ATOM	15	CG	LEU	1	2	35.203	-6.310	91.465	1.00	0.97
ATOM	16	CD1	LEU	1	2	35.397	-7.582	90.624	1.00	0.97
ATOM	17	CD2	LEU	1	2	36.445	-5.948	92.295	1.00	0.97
ATOM	18	N	THR	1	3	33.154	-2.414	89.990	1.00	4.97
ATOM	19	CA	THR	1	3	32.946	-1.389	89.006	1.00	4.97
ATOM	20	C	THR	1	3	33.539	-0.098	89.475	1.00	4.97
ATOM	21	O	THR	1	3	33.281	0.370	90.583	1.00	4.97
ATOM	22	CB	THR	1	3	31.496	-1.151	88.687	1.00	4.97
ATOM	23	OG1	THR	1	3	31.375	-0.248	87.598	1.00	4.97
ATOM	24	CG2	THR	1	3	30.792	-0.588	89.932	1.00	4.97
ATOM	25	N	PRO	1	4	34.334	0.496	88.629	1.00	1.53
ATOM	26	CA	PRO	1	4	34.970	1.734	88.985	1.00	1.53
ATOM	27	C	PRO	1	4	33.953	2.822	89.105	1.00	1.53
ATOM	28	O	PRO	1	4	32.935	2.768	88.416	1.00	1.53
ATOM	29	CB	PRO	1	4	36.021	1.984	87.906	1.00	1.53
ATOM	30	CG	PRO	1	4	36.397	0.567	87.435	1.00	1.53
ATOM	31	CD	PRO	1	4	35.129	-0.270	87.682	1.00	1.53
ATOM	32	N	THR	1	5	34.221	3.822	89.966	1.00	4.74
ATOM	33	CA	THR	1	5	33.280	4.873	90.217	1.00	4.74
ATOM	34	C	THR	1	5	32.996	5.653	88.973	1.00	4.74
ATOM	35	O	THR	1	5	31.839	5.946	88.679	1.00	4.74
ATOM	36	CB	THR	1	5	33.749	5.833	91.276	1.00	4.74
ATOM	37	OG1	THR	1	5	32.717	6.755	91.592	1.00	4.74
ATOM	38	CG2	THR	1	5	35.000	6.575	90.777	1.00	4.74
ATOM	39	N	LEU	1	6	34.042	5.976	88.189	1.00	0.89
ATOM	40	CA	LEU	1	6	33.888	6.778	87.008	1.00	0.89
ATOM	41	C	LEU	1	6	33.005	6.068	86.029	1.00	0.89
ATOM	42	O	LEU	1	6	32.203	6.696	85.338	1.00	0.89
ATOM	43	CB	LEU	1	6	35.231	7.060	86.306	1.00	0.89
ATOM	44	CG	LEU	1	6	35.101	7.915	85.031	1.00	0.89
ATOM	45	CD1	LEU	1	6	34.528	9.306	85.351	1.00	0.89
ATOM	46	CD2	LEU	1	6	36.436	7.988	84.273	1.00	0.89
ATOM	47	N	VAL	1	7	33.146	4.733	85.934	1.00	0.63
ATOM	48	CA	VAL	1	7	32.354	3.959	85.021	1.00	0.63

99/208

ATOM	49	C	VAL 1	7	30.930	4.080	85.438	1.00	0.63
ATOM	50	O	VAL 1	7	30.032	4.219	84.610	1.00	0.63
ATOM	51	CB	VAL 1	7	32.646	2.485	85.082	1.00	0.63
ATOM	52	CG1	VAL 1	7	31.739	1.778	84.061	1.00	0.63
ATOM	53	CG2	VAL 1	7	34.150	2.232	84.893	1.00	0.63
ATOM	54	N	SER 1	8	30.698	4.024	86.760	1.00	0.66
ATOM	55	CA	SER 1	8	29.369	4.077	87.284	1.00	0.66
ATOM	56	C	SER 1	8	28.753	5.387	86.910	1.00	0.66
ATOM	57	O	SER 1	8	27.579	5.432	86.546	1.00	0.66
ATOM	58	CB	SER 1	8	29.331	3.967	88.819	1.00	0.66
ATOM	59	OG	SER 1	8	29.819	2.698	89.229	1.00	0.66
ATOM	60	N	LEU 1	9	29.523	6.497	86.978	1.00	8.73
ATOM	61	CA	LEU 1	9	28.901	7.750	86.646	1.00	8.73
ATOM	62	C	LEU 1	9	28.462	7.675	85.232	1.00	8.73
ATOM	63	O	LEU 1	9	27.335	8.038	84.904	1.00	8.73
ATOM	64	CB	LEU 1	9	29.780	9.012	86.517	1.00	8.73
ATOM	65	CG	LEU 1	9	30.572	9.500	87.724	1.00	8.73
ATOM	66	CD1	LEU 1	9	29.685	9.772	88.945	1.00	8.73
ATOM	67	CD2	LEU 1	9	31.763	8.586	87.961	1.00	8.73
ATOM	68	N	LEU 1	10	29.363	7.182	84.363	1.00	1.17
ATOM	69	CA	LEU 1	10	29.124	7.190	82.952	1.00	1.17
ATOM	70	C	LEU 1	10	27.867	6.438	82.663	1.00	1.17
ATOM	71	O	LEU 1	10	27.061	6.863	81.837	1.00	1.17
ATOM	72	CB	LEU 1	10	30.291	6.589	82.144	1.00	1.17
ATOM	73	CG	LEU 1	10	31.600	7.406	82.258	1.00	1.17
ATOM	74	CD1	LEU 1	10	32.739	6.781	81.435	1.00	1.17
ATOM	75	CD2	LEU 1	10	31.372	8.887	81.913	1.00	1.17
ATOM	76	N	GLU 1	11	27.653	5.307	83.355	1.00	3.68
ATOM	77	CA	GLU 1	11	26.453	4.545	83.160	1.00	3.68
ATOM	78	C	GLU 1	11	25.296	5.429	83.496	1.00	3.68
ATOM	79	O	GLU 1	11	24.319	5.514	82.752	1.00	3.68
ATOM	80	CB	GLU 1	11	26.364	3.363	84.145	1.00	3.68
ATOM	81	CG	GLU 1	11	27.158	2.110	83.772	1.00	3.68
ATOM	82	CD	GLU 1	11	26.140	1.007	83.512	1.00	3.68
ATOM	83	OE1	GLU 1	11	25.188	0.896	84.330	1.00	3.68
ATOM	84	OE2	GLU 1	11	26.293	0.260	82.511	1.00	3.68
ATOM	85	N	VAL 1	12	25.395	6.135	84.635	1.00	0.75
ATOM	86	CA	VAL 1	12	24.309	6.939	85.107	1.00	0.75
ATOM	87	C	VAL 1	12	23.970	8.054	84.169	1.00	0.75
ATOM	88	O	VAL 1	12	22.797	8.283	83.880	1.00	0.75
ATOM	89	CB	VAL 1	12	24.598	7.561	86.442	1.00	0.75
ATOM	90	CG1	VAL 1	12	23.394	8.424	86.854	1.00	0.75
ATOM	91	CG2	VAL 1	12	24.934	6.439	87.440	1.00	0.75
ATOM	92	N	ILE 1	13	24.984	8.784	83.664	1.00	4.56
ATOM	93	CA	ILE 1	13	24.694	9.920	82.836	1.00	4.56
ATOM	94	C	ILE 1	13	24.234	9.610	81.445	1.00	4.56
ATOM	95	O	ILE 1	13	23.698	10.497	80.784	1.00	4.56
ATOM	96	CB	ILE 1	13	25.744	11.011	82.766	1.00	4.56
ATOM	97	CG1	ILE 1	13	27.064	10.605	82.098	1.00	4.56

100/208

ATOM	98	CG2 ILE 1	13	25.959	11.490	84.213	1.00	4.56
ATOM	99	CD1 ILE 1	13	28.035	9.910	83.035	1.00	4.56
ATOM	100	N GLU 1	14	24.471	8.384	80.928	1.00	2.30
ATOM	101	CA GLU 1	14	24.078	8.151	79.566	1.00	2.30
ATOM	102	C GLU 1	14	22.611	8.405	79.384	1.00	2.30
ATOM	103	O GLU 1	14	21.774	8.069	80.220	1.00	2.30
ATOM	104	CB GLU 1	14	24.485	6.783	78.994	1.00	2.30
ATOM	105	CG GLU 1	14	24.341	6.743	77.471	1.00	2.30
ATOM	106	CD GLU 1	14	25.404	5.808	76.924	1.00	2.30
ATOM	107	OE1 GLU 1	14	26.589	6.006	77.303	1.00	2.30
ATOM	108	OE2 GLU 1	14	25.060	4.899	76.122	1.00	2.30
ATOM	109	N PRO 1	15	22.304	9.030	78.278	1.00	6.71
ATOM	110	CA PRO 1	15	20.949	9.443	78.025	1.00	6.71
ATOM	111	C PRO 1	15	20.014	8.313	77.771	1.00	6.71
ATOM	112	O PRO 1	15	20.454	7.242	77.356	1.00	6.71
ATOM	113	CB PRO 1	15	21.022	10.438	76.870	1.00	6.71
ATOM	114	CG PRO 1	15	22.432	11.038	76.998	1.00	6.71
ATOM	115	CD PRO 1	15	23.264	9.918	77.643	1.00	6.71
ATOM	116	N GLU 1	16	18.712	8.539	78.032	1.00	3.50
ATOM	117	CA GLU 1	16	17.726	7.533	77.798	1.00	3.50
ATOM	118	C GLU 1	16	17.577	7.447	76.316	1.00	3.50
ATOM	119	O GLU 1	16	18.023	8.329	75.584	1.00	3.50
ATOM	120	CB GLU 1	16	16.348	7.856	78.404	1.00	3.50
ATOM	121	CG GLU 1	16	15.723	9.143	77.862	1.00	3.50
ATOM	122	CD GLU 1	16	14.375	9.333	78.542	1.00	3.50
ATOM	123	OE1 GLU 1	16	14.007	8.465	79.378	1.00	3.50
ATOM	124	OE2 GLU 1	16	13.695	10.348	78.235	1.00	3.50
ATOM	125	N VAL 1	17	16.953	6.359	75.831	1.00	1.33
ATOM	126	CA VAL 1	17	16.815	6.185	74.417	1.00	1.33
ATOM	127	C VAL 1	17	16.046	7.322	73.826	1.00	1.33
ATOM	128	O VAL 1	17	15.108	7.846	74.423	1.00	1.33
ATOM	129	CB VAL 1	17	16.115	4.914	74.029	1.00	1.33
ATOM	130	CG1 VAL 1	17	15.809	4.956	72.526	1.00	1.33
ATOM	131	CG2 VAL 1	17	17.015	3.732	74.408	1.00	1.33
ATOM	132	N LEU 1	18	16.453	7.724	72.607	1.00	6.49
ATOM	133	CA LEU 1	18	15.863	8.817	71.889	1.00	6.49
ATOM	134	C LEU 1	18	15.010	8.266	70.788	1.00	6.49
ATOM	135	O LEU 1	18	15.418	7.345	70.083	1.00	6.49
ATOM	136	CB LEU 1	18	16.940	9.683	71.217	1.00	6.49
ATOM	137	CG LEU 1	18	16.413	10.883	70.418	1.00	6.49
ATOM	138	CD1 LEU 1	18	15.769	11.940	71.329	1.00	6.49
ATOM	139	CD2 LEU 1	18	17.523	11.442	69.514	1.00	6.49
ATOM	140	N TYR 1	19	13.795	8.830	70.609	1.00	0.75
ATOM	141	CA TYR 1	19	12.907	8.372	69.575	1.00	0.75
ATOM	142	C TYR 1	19	12.967	9.322	68.419	1.00	0.75
ATOM	143	O TYR 1	19	13.101	10.533	68.592	1.00	0.75
ATOM	144	CB TYR 1	19	11.432	8.284	70.007	1.00	0.75
ATOM	145	CG TYR 1	19	11.317	7.194	71.016	1.00	0.75
ATOM	146	CD1 TYR 1	19	11.565	7.440	72.347	1.00	0.75

SUBSTITUTE SHEET (RULE 26)

101/208

ATOM	147	CD2 TYR 1 19	10.970	5.920	70.627	1.00	0.75
ATOM	148	CE1 TYR 1 19	11.468	6.431	73.276	1.00	0.75
ATOM	149	CE2 TYR 1 19	10.874	4.907	71.552	1.00	0.75
ATOM	150	CZ TYR 1 19	11.125	5.162	72.878	1.00	0.75
ATOM	151	OH TYR 1 19	11.032	4.124	73.830	1.00	0.75
ATOM	152	N ALA 1 20	12.923	8.766	67.192	1.00	1.03
ATOM	153	CA ALA 1 20	12.957	9.542	65.982	1.00	1.03
ATOM	154	C ALA 1 20	11.661	10.258	65.768	1.00	1.03
ATOM	155	O ALA 1 20	11.626	11.345	65.191	1.00	1.03
ATOM	156	CB ALA 1 20	13.237	8.691	64.730	1.00	1.03
ATOM	157	N GLY 1 21	10.549	9.642	66.210	1.00	0.75
ATOM	158	CA GLY 1 21	9.268	10.244	66.005	1.00	0.75
ATOM	159	C GLY 1 21	8.897	10.016	64.574	1.00	0.75
ATOM	160	O GLY 1 21	8.194	10.836	63.983	1.00	0.75
ATOM	161	N TYR 1 22	9.368	8.905	63.959	1.00	4.21
ATOM	162	CA TYR 1 22	9.008	8.766	62.577	1.00	4.21
ATOM	163	C TYR 1 22	7.659	8.129	62.432	1.00	4.21
ATOM	164	O TYR 1 22	7.187	7.412	63.313	1.00	4.21
ATOM	165	CB TYR 1 22	10.036	8.080	61.636	1.00	4.21
ATOM	166	CG TYR 1 22	9.989	6.587	61.596	1.00	4.21
ATOM	167	CD1 TYR 1 22	8.946	5.944	60.960	1.00	4.21
ATOM	168	CD2 TYR 1 22	11.165	5.887	61.738	1.00	4.21
ATOM	169	CE1 TYR 1 22	9.008	4.616	60.613	1.00	4.21
ATOM	170	CE2 TYR 1 22	11.255	4.573	61.345	1.00	4.21
ATOM	171	CZ TYR 1 22	10.174	3.924	60.806	1.00	4.21
ATOM	172	OH TYR 1 22	10.274	2.570	60.421	1.00	4.21
ATOM	173	N ASP 1 23	6.996	8.403	61.290	1.00	3.58
ATOM	174	CA ASP 1 23	5.649	7.950	61.068	1.00	3.58
ATOM	175	C ASP 1 23	5.491	6.457	61.014	1.00	3.58
ATOM	176	O ASP 1 23	4.768	5.874	61.823	1.00	3.58
ATOM	177	CB ASP 1 23	5.060	8.515	59.762	1.00	3.58
ATOM	178	CG ASP 1 23	3.559	8.254	59.744	1.00	3.58
ATOM	179	OD1 ASP 1 23	3.041	7.660	60.727	1.00	3.58
ATOM	180	OD2 ASP 1 23	2.909	8.650	58.740	1.00	3.58
ATOM	181	N SER 1 24	6.185	5.797	60.069	1.00	3.81
ATOM	182	CA SER 1 24	6.117	4.371	59.899	1.00	3.81
ATOM	183	C SER 1 24	4.843	3.956	59.222	1.00	3.81
ATOM	184	O SER 1 24	4.821	2.977	58.478	1.00	3.81
ATOM	185	CB SER 1 24	6.208	3.608	61.231	1.00	3.81
ATOM	186	OG SER 1 24	6.138	2.209	60.997	1.00	3.81
ATOM	187	N SER 1 25	3.760	4.735	59.402	1.00	3.40
ATOM	188	CA SER 1 25	2.488	4.381	58.834	1.00	3.40
ATOM	189	C SER 1 25	2.578	4.438	57.345	1.00	3.40
ATOM	190	O SER 1 25	1.996	3.609	56.647	1.00	3.40
ATOM	191	CB SER 1 25	1.358	5.334	59.260	1.00	3.40
ATOM	192	OG SER 1 25	0.131	4.932	58.670	1.00	3.40
ATOM	193	N VAL 1 26	3.332	5.425	56.826	1.00	1.09
ATOM	194	CA VAL 1 26	3.411	5.643	55.409	1.00	1.09
ATOM	195	C VAL 1 26	4.639	4.982	54.864	1.00	1.09

SUBSTITUTE SHEET (RULE 26)

102/208

ATOM	196	O	VAL 1	26	5.579	4.677	55.597	1.00	1.09
ATOM	197	CB	VAL 1	26	3.478	7.107	55.066	1.00	1.09
ATOM	198	CG1	VAL 1	26	3.569	7.286	53.541	1.00	1.09
ATOM	199	CG2	VAL 1	26	2.258	7.800	55.694	1.00	1.09
ATOM	200	N	PRO 1	27	4.631	4.714	53.582	1.00	1.62
ATOM	201	CA	PRO 1	27	5.779	4.108	52.974	1.00	1.62
ATOM	202	C	PRO 1	27	6.940	5.046	53.001	1.00	1.62
ATOM	203	O	PRO 1	27	6.802	6.193	52.577	1.00	1.62
ATOM	204	CB	PRO 1	27	5.336	3.662	51.583	1.00	1.62
ATOM	205	CG	PRO 1	27	3.831	3.388	51.767	1.00	1.62
ATOM	206	CD	PRO 1	27	3.401	4.330	52.906	1.00	1.62
ATOM	207	N	ASP 1	28	8.104	4.559	53.467	1.00	1.30
ATOM	208	CA	ASP 1	28	9.254	5.398	53.617	1.00	1.30
ATOM	209	C	ASP 1	28	9.928	5.629	52.304	1.00	1.30
ATOM	210	O	ASP 1	28	10.293	4.688	51.600	1.00	1.30
ATOM	211	CB	ASP 1	28	10.315	4.781	54.543	1.00	1.30
ATOM	212	CG	ASP 1	28	9.737	4.660	55.947	1.00	1.30
ATOM	213	OD1	ASP 1	28	8.605	5.166	56.170	1.00	1.30
ATOM	214	OD2	ASP 1	28	10.423	4.057	56.815	1.00	1.30
ATOM	215	N	SER 1	29	10.124	6.911	51.948	1.00	3.54
ATOM	216	CA	SER 1	29	10.824	7.216	50.739	1.00	3.54
ATOM	217	C	SER 1	29	12.225	7.538	51.142	1.00	3.54
ATOM	218	O	SER 1	29	12.521	7.686	52.327	1.00	3.54
ATOM	219	CB	SER 1	29	10.246	8.412	49.973	1.00	3.54
ATOM	220	OG	SER 1	29	11.001	8.632	48.793	1.00	3.54
ATOM	221	N	THR 1	30	13.138	7.644	50.160	1.00	4.86
ATOM	222	CA	THR 1	30	14.509	7.906	50.481	1.00	4.86
ATOM	223	C	THR 1	30	14.641	9.237	51.156	1.00	4.86
ATOM	224	O	THR 1	30	15.323	9.357	52.173	1.00	4.86
ATOM	225	CB	THR 1	30	15.399	7.895	49.269	1.00	4.86
ATOM	226	OG1	THR 1	30	16.754	8.080	49.653	1.00	4.86
ATOM	227	CG2	THR 1	30	14.956	9.001	48.295	1.00	4.86
ATOM	228	N	TRP 1	31	13.976	10.275	50.616	1.00	6.14
ATOM	229	CA	TRP 1	31	14.080	11.589	51.186	1.00	6.14
ATOM	230	C	TRP 1	31	13.464	11.621	52.544	1.00	6.14
ATOM	231	O	TRP 1	31	14.005	12.236	53.461	1.00	6.14
ATOM	232	CB	TRP 1	31	13.359	12.670	50.367	1.00	6.14
ATOM	233	CG	TRP 1	31	11.901	12.359	50.163	1.00	6.14
ATOM	234	CD1	TRP 1	31	11.320	11.152	49.924	1.00	6.14
ATOM	235	CD2	TRP 1	31	10.830	13.306	50.286	1.00	6.14
ATOM	236	NE1	TRP 1	31	9.956	11.290	49.846	1.00	6.14
ATOM	237	CE2	TRP 1	31	9.639	12.612	50.074	1.00	6.14
ATOM	238	CE3	TRP 1	31	10.836	14.642	50.560	1.00	6.14
ATOM	239	CZ2	TRP 1	31	8.433	13.248	50.122	1.00	6.14
ATOM	240	CZ3	TRP 1	31	9.619	15.283	50.606	1.00	6.14
ATOM	241	CH2	TRP 1	31	8.440	14.600	50.387	1.00	6.14
ATOM	242	N	ARG 1	32	12.303	10.961	52.705	1.00	4.31
ATOM	243	CA	ARG 1	32	11.616	10.989	53.964	1.00	4.31
ATOM	244	C	ARG 1	32	12.464	10.336	55.006	1.00	4.31

SUBSTITUTE SHEET (RULE 26)



103/208

ATOM	245	O	ARG 1	32	12.542	10.805	56.141	1.00	4.31
ATOM	246	CB	ARG 1	32	10.270	10.243	53.942	1.00	4.31
ATOM	247	CG	ARG 1	32	9.191	10.930	53.104	1.00	4.31
ATOM	248	CD	ARG 1	32	7.797	10.331	53.305	1.00	4.31
ATOM	249	NE	ARG 1	32	7.321	10.755	54.653	1.00	4.31
ATOM	250	CZ	ARG 1	32	6.177	10.226	55.177	1.00	4.31
ATOM	251	NH1	ARG 1	32	5.742	10.626	56.408	1.00	4.31
ATOM	252	NH2	ARG 1	32	5.469	9.295	54.473	1.00	4.31
ATOM	253	N	ILE 1	33	13.125	9.224	54.644	1.00	3.71
ATOM	254	CA	ILE 1	33	13.940	8.530	55.594	1.00	3.71
ATOM	255	C	ILE 1	33	15.061	9.402	56.059	1.00	3.71
ATOM	256	O	ILE 1	33	15.351	9.472	57.252	1.00	3.71
ATOM	257	CB	ILE 1	33	14.560	7.284	55.032	1.00	3.71
ATOM	258	CG1	ILE 1	33	13.474	6.250	54.703	1.00	3.71
ATOM	259	CG2	ILE 1	33	15.600	6.777	56.045	1.00	3.71
ATOM	260	CD1	ILE 1	33	12.707	5.788	55.940	1.00	3.71
ATOM	261	N	MET 1	34	15.725	10.105	55.129	1.00	6.71
ATOM	262	CA	MET 1	34	16.838	10.910	55.535	1.00	6.71
ATOM	263	C	MET 1	34	16.356	12.005	56.428	1.00	6.71
ATOM	264	O	MET 1	34	17.008	12.349	57.413	1.00	6.71
ATOM	265	CB	MET 1	34	17.596	11.530	54.353	1.00	6.71
ATOM	266	CG	MET 1	34	18.982	12.038	54.748	1.00	6.71
ATOM	267	SD	MET 1	34	20.190	10.734	55.128	1.00	6.71
ATOM	268	CE	MET 1	34	21.536	11.890	55.515	1.00	6.71
ATOM	269	N	THR 1	35	15.182	12.578	56.104	1.00	0.49
ATOM	270	CA	THR 1	35	14.647	13.643	56.897	1.00	0.49
ATOM	271	C	THR 1	35	14.395	13.141	58.285	1.00	0.49
ATOM	272	O	THR 1	35	14.699	13.826	59.260	1.00	0.49
ATOM	273	CB	THR 1	35	13.344	14.164	56.367	1.00	0.49
ATOM	274	OG1	THR 1	35	13.515	14.665	55.049	1.00	0.49
ATOM	275	CG2	THR 1	35	12.845	15.282	57.299	1.00	0.49
ATOM	276	N	THR 1	36	13.835	11.922	58.418	1.00	4.72
ATOM	277	CA	THR 1	36	13.543	11.426	59.732	1.00	4.72
ATOM	278	C	THR 1	36	14.811	11.197	60.490	1.00	4.72
ATOM	279	O	THR 1	36	14.868	11.419	61.698	1.00	4.72
ATOM	280	CB	THR 1	36	12.757	10.144	59.749	1.00	4.72
ATOM	281	OG1	THR 1	36	12.240	9.916	61.052	1.00	4.72
ATOM	282	CG2	THR 1	36	13.674	8.976	59.355	1.00	4.72
ATOM	283	N	LEU 1	37	15.865	10.722	59.805	1.00	6.67
ATOM	284	CA	LEU 1	37	17.095	10.476	60.496	1.00	6.67
ATOM	285	C	LEU 1	37	17.709	11.770	60.945	1.00	6.67
ATOM	286	O	LEU 1	37	18.377	11.827	61.976	1.00	6.67
ATOM	287	CB	LEU 1	37	18.104	9.650	59.689	1.00	6.67
ATOM	288	CG	LEU 1	37	19.264	9.170	60.574	1.00	6.67
ATOM	289	CD1	LEU 1	37	18.732	8.452	61.824	1.00	6.67
ATOM	290	CD2	LEU 1	37	20.215	8.261	59.788	1.00	6.67
ATOM	291	N	ASN 1	38	17.520	12.851	60.164	1.00	0.62
ATOM	292	CA	ASN 1	38	18.044	14.132	60.547	1.00	0.62
ATOM	293	C	ASN 1	38	17.355	14.597	61.793	1.00	0.62

104/208

ATOM	294	O	ASN	1	38	17.978	15.197	62.668	1.00	0.62
ATOM	295	CB	ASN	1	38	17.840	15.217	59.474	1.00	0.62
ATOM	296	CG	ASN	1	38	18.787	14.931	58.315	1.00	0.62
ATOM	297	OD1	ASN	1	38	19.823	14.291	58.486	1.00	0.62
ATOM	298	ND2	ASN	1	38	18.427	15.428	57.101	1.00	0.62
ATOM	299	N	MET	1	39	16.036	14.337	61.896	1.00	3.81
ATOM	300	CA	MET	1	39	15.265	14.746	63.037	1.00	3.81
ATOM	301	C	MET	1	39	15.797	14.033	64.238	1.00	3.81
ATOM	302	O	MET	1	39	15.937	14.618	65.312	1.00	3.81
ATOM	303	CB	MET	1	39	13.779	14.373	62.907	1.00	3.81
ATOM	304	CG	MET	1	39	13.070	15.075	61.746	1.00	3.81
ATOM	305	SD	MET	1	39	11.311	14.649	61.572	1.00	3.81
ATOM	306	CE	MET	1	39	11.071	15.588	60.036	1.00	3.81
ATOM	307	N	LEU	1	40	16.109	12.735	64.081	1.00	0.61
ATOM	308	CA	LEU	1	40	16.635	11.963	65.166	1.00	0.61
ATOM	309	C	LEU	1	40	17.956	12.559	65.555	1.00	0.61
ATOM	310	O	LEU	1	40	18.264	12.708	66.737	1.00	0.61
ATOM	311	CB	LEU	1	40	16.868	10.496	64.762	1.00	0.61
ATOM	312	CG	LEU	1	40	17.439	9.607	65.880	1.00	0.61
ATOM	313	CD1	LEU	1	40	16.465	9.504	67.066	1.00	0.61
ATOM	314	CD2	LEU	1	40	17.853	8.232	65.332	1.00	0.61
ATOM	315	N	GLY	1	41	18.762	12.947	64.550	1.00	0.41
ATOM	316	CA	GLY	1	41	20.063	13.501	64.797	1.00	0.41
ATOM	317	C	GLY	1	41	19.947	14.758	65.600	1.00	0.41
ATOM	318	O	GLY	1	41	20.773	15.023	66.472	1.00	0.41
ATOM	319	N	GLY	1	42	18.926	15.584	65.309	1.00	0.36
ATOM	320	CA	GLY	1	42	18.765	16.812	66.031	1.00	0.36
ATOM	321	C	GLY	1	42	18.514	16.504	67.473	1.00	0.36
ATOM	322	O	GLY	1	42	19.052	17.165	68.359	1.00	0.36
ATOM	323	N	ARG	1	43	17.667	15.491	67.742	1.00	3.86
ATOM	324	CA	ARG	1	43	17.347	15.134	69.095	1.00	3.86
ATOM	325	C	ARG	1	43	18.549	14.575	69.790	1.00	3.86
ATOM	326	O	ARG	1	43	18.742	14.794	70.983	1.00	3.86
ATOM	327	CB	ARG	1	43	16.243	14.074	69.213	1.00	3.86
ATOM	328	CG	ARG	1	43	14.859	14.528	68.756	1.00	3.86
ATOM	329	CD	ARG	1	43	13.772	13.521	69.131	1.00	3.86
ATOM	330	NE	ARG	1	43	12.525	13.909	68.420	1.00	3.86
ATOM	331	CZ	ARG	1	43	12.362	13.517	67.124	1.00	3.86
ATOM	332	NH1	ARG	1	43	11.193	13.774	66.469	1.00	3.86
ATOM	333	NH2	ARG	1	43	13.380	12.867	66.488	1.00	3.86
ATOM	334	N	GLN	1	44	19.371	13.792	69.069	1.00	1.14
ATOM	335	CA	GLN	1	44	20.545	13.211	69.655	1.00	1.14
ATOM	336	C	GLN	1	44	21.563	14.265	69.967	1.00	1.14
ATOM	337	O	GLN	1	44	22.303	14.153	70.944	1.00	1.14
ATOM	338	CB	GLN	1	44	21.202	12.148	68.759	1.00	1.14
ATOM	339	CG	GLN	1	44	20.322	10.909	68.574	1.00	1.14
ATOM	340	CD	GLN	1	44	21.060	9.924	67.679	1.00	1.14
ATOM	341	OE1	GLN	1	44	20.499	9.396	66.720	1.00	1.14
ATOM	342	NE2	GLN	1	44	22.351	9.655	68.008	1.00	1.14

SUBSTITUTE SHEET (RULE 26)

105/208

ATOM	343	N	VAL	1	45	21.640	15.316	69.129	1.00	0.68
ATOM	344	CA	VAL	1	45	22.607	16.356	69.340	1.00	0.68
ATOM	345	C	VAL	1	45	22.347	17.012	70.657	1.00	0.68
ATOM	346	O	VAL	1	45	23.276	17.273	71.419	1.00	0.68
ATOM	347	CB	VAL	1	45	22.551	17.427	68.290	1.00	0.68
ATOM	348	CG1	VAL	1	45	23.548	18.534	68.669	1.00	0.68
ATOM	349	CG2	VAL	1	45	22.829	16.787	66.919	1.00	0.68
ATOM	350	N	ILE	1	46	21.066	17.292	70.968	1.00	3.68
ATOM	351	CA	ILE	1	46	20.767	17.932	72.216	1.00	3.68
ATOM	352	C	ILE	1	46	21.144	16.999	73.323	1.00	3.68
ATOM	353	O	ILE	1	46	21.656	17.416	74.360	1.00	3.68
ATOM	354	CB	ILE	1	46	19.320	18.308	72.383	1.00	3.68
ATOM	355	CG1	ILE	1	46	19.163	19.287	73.559	1.00	3.68
ATOM	356	CG2	ILE	1	46	18.487	17.028	72.547	1.00	3.68
ATOM	357	CD1	ILE	1	46	17.789	19.952	73.617	1.00	3.68
ATOM	358	N	ALA	1	47	20.910	15.691	73.123	1.00	0.54
ATOM	359	CA	ALA	1	47	21.221	14.727	74.136	1.00	0.54
ATOM	360	C	ALA	1	47	22.695	14.748	74.397	1.00	0.54
ATOM	361	O	ALA	1	47	23.130	14.677	75.546	1.00	0.54
ATOM	362	CB	ALA	1	47	20.845	13.293	73.726	1.00	0.54
ATOM	363	N	ALA	1	48	23.505	14.854	73.327	1.00	0.69
ATOM	364	CA	ALA	1	48	24.934	14.846	73.450	1.00	0.69
ATOM	365	C	ALA	1	48	25.414	16.025	74.239	1.00	0.69
ATOM	366	O	ALA	1	48	26.303	15.890	75.078	1.00	0.69
ATOM	367	CB	ALA	1	48	25.648	14.887	72.089	1.00	0.69
ATOM	368	N	VAL	1	49	24.846	17.222	73.992	1.00	4.14
ATOM	369	CA	VAL	1	49	25.308	18.380	74.705	1.00	4.14
ATOM	370	C	VAL	1	49	24.997	18.224	76.160	1.00	4.14
ATOM	371	O	VAL	1	49	25.816	18.556	77.015	1.00	4.14
ATOM	372	CB	VAL	1	49	24.685	19.680	74.258	1.00	4.14
ATOM	373	CG1	VAL	1	49	25.020	19.902	72.779	1.00	4.14
ATOM	374	CG2	VAL	1	49	23.180	19.682	74.561	1.00	4.14
ATOM	375	N	LYS	1	50	23.797	17.703	76.478	1.00	4.12
ATOM	376	CA	LYS	1	50	23.385	17.556	77.843	1.00	4.12
ATOM	377	C	LYS	1	50	24.303	16.597	78.529	1.00	4.12
ATOM	378	O	LYS	1	50	24.723	16.823	79.663	1.00	4.12
ATOM	379	CB	LYS	1	50	21.956	17.000	77.969	1.00	4.12
ATOM	380	CG	LYS	1	50	20.885	17.949	77.427	1.00	4.12
ATOM	381	CD	LYS	1	50	19.523	17.283	77.219	1.00	4.12
ATOM	382	CE	LYS	1	50	18.819	16.903	78.523	1.00	4.12
ATOM	383	NZ	LYS	1	50	18.315	18.118	79.200	1.00	4.12
ATOM	384	N	TRP	1	51	24.653	15.500	77.835	1.00	1.08
ATOM	385	CA	TRP	1	51	25.499	14.479	78.378	1.00	1.08
ATOM	386	C	TRP	1	51	26.840	15.056	78.713	1.00	1.08
ATOM	387	O	TRP	1	51	27.404	14.777	79.769	1.00	1.08
ATOM	388	CB	TRP	1	51	25.696	13.328	77.372	1.00	1.08
ATOM	389	CG	TRP	1	51	26.619	12.207	77.794	1.00	1.08
ATOM	390	CD1	TRP	1	51	26.426	11.208	78.703	1.00	1.08
ATOM	391	CD2	TRP	1	51	27.845	11.903	77.112	1.00	1.08

106/208

ATOM	392	NE1 TRP	1	51	27.477	10.322	78.658	1.00	1.08
ATOM	393	CE2 TRP	1	51	28.351	10.731	77.673	1.00	1.08
ATOM	394	CE3 TRP	1	51	28.486	12.539	76.089	1.00	1.08
ATOM	395	CZ2 TRP	1	51	29.515	10.176	77.220	1.00	1.08
ATOM	396	CZ3 TRP	1	51	29.659	11.977	75.634	1.00	1.08
ATOM	397	CH2 TRP	1	51	30.163	10.818	76.187	1.00	1.08
ATOM	398	N ALA	1	52	27.369	15.915	77.827	1.00	0.96
ATOM	399	CA ALA	1	52	28.672	16.497	78.001	1.00	0.96
ATOM	400	C ALA	1	52	28.739	17.346	79.234	1.00	0.96
ATOM	401	O ALA	1	52	29.788	17.447	79.869	1.00	0.96
ATOM	402	CB ALA	1	52	29.092	17.377	76.811	1.00	0.96
ATOM	403	N LYS	1	53	27.624	18.005	79.593	1.00	1.49
ATOM	404	CA LYS	1	53	27.607	18.862	80.744	1.00	1.49
ATOM	405	C LYS	1	53	27.885	18.038	81.967	1.00	1.49
ATOM	406	O LYS	1	53	28.537	18.496	82.902	1.00	1.49
ATOM	407	CB LYS	1	53	26.241	19.541	80.934	1.00	1.49
ATOM	408	CG LYS	1	53	25.853	20.448	79.763	1.00	1.49
ATOM	409	CD LYS	1	53	24.376	20.846	79.760	1.00	1.49
ATOM	410	CE LYS	1	53	23.985	21.753	78.592	1.00	1.49
ATOM	411	NZ LYS	1	53	22.544	22.086	78.671	1.00	1.49
ATOM	412	N ALA	1	54	27.331	16.813	82.003	1.00	1.47
ATOM	413	CA ALA	1	54	27.477	15.863	83.072	1.00	1.47
ATOM	414	C ALA	1	54	28.807	15.162	83.114	1.00	1.47
ATOM	415	O ALA	1	54	29.223	14.688	84.171	1.00	1.47
ATOM	416	CB ALA	1	54	26.400	14.766	83.028	1.00	1.47
ATOM	417	N ILE	1	55	29.487	15.027	81.957	1.00	4.27
ATOM	418	CA ILE	1	55	30.697	14.250	81.896	1.00	4.27
ATOM	419	C ILE	1	55	31.835	14.871	82.643	1.00	4.27
ATOM	420	O ILE	1	55	32.224	16.013	82.407	1.00	4.27
ATOM	421	CB ILE	1	55	31.139	13.951	80.492	1.00	4.27
ATOM	422	CG1 ILE	1	55	32.287	12.928	80.492	1.00	4.27
ATOM	423	CG2 ILE	1	55	31.470	15.278	79.796	1.00	4.27
ATOM	424	CD1 ILE	1	55	32.586	12.351	79.109	1.00	4.27
ATOM	425	N PRO	1	56	32.400	14.113	83.548	1.00	6.47
ATOM	426	CA PRO	1	56	33.455	14.586	84.395	1.00	6.47
ATOM	427	C PRO	1	56	34.624	15.142	83.639	1.00	6.47
ATOM	428	O PRO	1	56	35.175	14.461	82.775	1.00	6.47
ATOM	429	CB PRO	1	56	33.793	13.420	85.332	1.00	6.47
ATOM	430	CG PRO	1	56	33.206	12.179	84.629	1.00	6.47
ATOM	431	CD PRO	1	56	32.028	12.733	83.810	1.00	6.47
ATOM	432	N GLY	1	57	35.005	16.395	83.964	1.00	0.90
ATOM	433	CA GLY	1	57	36.155	17.046	83.406	1.00	0.90
ATOM	434	C GLY	1	57	35.842	17.885	82.201	1.00	0.90
ATOM	435	O GLY	1	57	36.558	18.839	81.906	1.00	0.90
ATOM	436	N PHE	1	58	34.753	17.572	81.480	1.00	1.63
ATOM	437	CA PHE	1	58	34.449	18.259	80.254	1.00	1.63
ATOM	438	C PHE	1	58	34.130	19.708	80.487	1.00	1.63
ATOM	439	O PHE	1	58	34.602	20.583	79.763	1.00	1.63
ATOM	440	CB PHE	1	58	33.255	17.606	79.532	1.00	1.63

107/208

ATOM	441	CG	PHE	1	58	33.258	17.977	78.087	1.00	1.63
ATOM	442	CD1	PHE	1	58	34.096	17.320	77.213	1.00	1.63
ATOM	443	CD2	PHE	1	58	32.309	18.831	77.576	1.00	1.63
ATOM	444	CE1	PHE	1	58	34.027	17.553	75.860	1.00	1.63
ATOM	445	CE2	PHE	1	58	32.233	19.067	76.223	1.00	1.63
ATOM	446	CZ	PHE	1	58	33.094	18.430	75.363	1.00	1.63
ATOM	447	N	ARG	1	59	33.345	20.002	81.538	1.00	3.96
ATOM	448	CA	ARG	1	59	32.897	21.339	81.821	1.00	3.96
ATOM	449	C	ARG	1	59	34.060	22.230	82.134	1.00	3.96
ATOM	450	O	ARG	1	59	33.975	23.446	81.976	1.00	3.96
ATOM	451	CB	ARG	1	59	31.901	21.413	82.993	1.00	3.96
ATOM	452	CG	ARG	1	59	32.454	20.929	84.335	1.00	3.96
ATOM	453	CD	ARG	1	59	31.399	20.919	85.444	1.00	3.96
ATOM	454	NE	ARG	1	59	32.051	20.436	86.693	1.00	3.96
ATOM	455	CZ	ARG	1	59	32.659	21.326	87.530	1.00	3.96
ATOM	456	NH1	ARG	1	59	33.256	20.887	88.677	1.00	3.96
ATOM	457	NH2	ARG	1	59	32.665	22.656	87.224	1.00	3.96
ATOM	458	N	ASN	1	60	35.160	21.640	82.632	1.00	1.96
ATOM	459	CA	ASN	1	60	36.355	22.344	83.008	1.00	1.96
ATOM	460	C	ASN	1	60	37.037	22.967	81.824	1.00	1.96
ATOM	461	O	ASN	1	60	37.734	23.971	81.961	1.00	1.96
ATOM	462	CB	ASN	1	60	37.373	21.425	83.699	1.00	1.96
ATOM	463	CG	ASN	1	60	36.744	20.971	85.008	1.00	1.96
ATOM	464	OD1	ASN	1	60	37.173	19.989	85.611	1.00	1.96
ATOM	465	ND2	ASN	1	60	35.687	21.700	85.455	1.00	1.96
ATOM	466	N	LEU	1	61	36.887	22.352	80.636	1.00	3.77
ATOM	467	CA	LEU	1	61	37.464	22.809	79.400	1.00	3.77
ATOM	468	C	LEU	1	61	36.970	24.195	79.135	1.00	3.77
ATOM	469	O	LEU	1	61	35.922	24.604	79.629	1.00	3.77
ATOM	470	CB	LEU	1	61	36.933	22.006	78.192	1.00	3.77
ATOM	471	CG	LEU	1	61	37.348	20.524	78.084	1.00	3.77
ATOM	472	CD1	LEU	1	61	38.702	20.360	77.389	1.00	3.77
ATOM	473	CD2	LEU	1	61	37.318	19.825	79.450	1.00	3.77
ATOM	474	N	HIS	1	62	37.728	24.956	78.323	1.00	0.83
ATOM	475	CA	HIS	1	62	37.312	26.273	77.944	1.00	0.83
ATOM	476	C	HIS	1	62	36.042	26.055	77.181	1.00	0.83
ATOM	477	O	HIS	1	62	35.859	25.014	76.553	1.00	0.83
ATOM	478	CB	HIS	1	62	38.329	26.959	77.014	1.00	0.83
ATOM	479	CG	HIS	1	62	38.028	28.396	76.709	1.00	0.83
ATOM	480	ND1	HIS	1	62	37.075	28.811	75.807	1.00	0.83
ATOM	481	CD2	HIS	1	62	38.621	29.530	77.172	1.00	0.83
ATOM	482	CE1	HIS	1	62	37.135	30.166	75.770	1.00	0.83
ATOM	483	NE2	HIS	1	62	38.059	30.648	76.582	1.00	0.83
ATOM	484	N	LEU	1	63	35.124	27.040	77.217	1.00	6.44
ATOM	485	CA	LEU	1	63	33.841	26.895	76.589	1.00	6.44
ATOM	486	C	LEU	1	63	34.012	26.678	75.119	1.00	6.44
ATOM	487	O	LEU	1	63	33.338	25.838	74.524	1.00	6.44
ATOM	488	CB	LEU	1	63	32.960	28.144	76.769	1.00	6.44
ATOM	489	CG	LEU	1	63	31.576	28.033	76.105	1.00	6.44

SUBSTITUTE SHEET (RULE 26)

108/208

ATOM	490	CD1 LEU 1	63	30.730	26.927	76.756	1.00	6.44
ATOM	491	CD2 LEU 1	63	30.858	29.392	76.080	1.00	6.44
ATOM	492	N ASP 1	64	34.939	27.426	74.496	1.00	0.59
ATOM	493	CA ASP 1	64	35.142	27.315	73.083	1.00	0.59
ATOM	494	C ASP 1	64	35.587	25.925	72.762	1.00	0.59
ATOM	495	O ASP 1	64	35.194	25.356	71.746	1.00	0.59
ATOM	496	CB ASP 1	64	36.215	28.286	72.561	1.00	0.59
ATOM	497	CG ASP 1	64	35.652	29.697	72.655	1.00	0.59
ATOM	498	OD1 ASP 1	64	34.419	29.830	72.879	1.00	0.59
ATOM	499	OD2 ASP 1	64	36.446	30.663	72.499	1.00	0.59
ATOM	500	N ASP 1	65	36.439	25.343	73.622	1.00	2.31
ATOM	501	CA ASP 1	65	36.945	24.022	73.393	1.00	2.31
ATOM	502	C ASP 1	65	35.824	23.033	73.448	1.00	2.31
ATOM	503	O ASP 1	65	35.732	22.133	72.615	1.00	2.31
ATOM	504	CB ASP 1	65	37.961	23.605	74.466	1.00	2.31
ATOM	505	CG ASP 1	65	39.139	24.565	74.380	1.00	2.31
ATOM	506	OD1 ASP 1	65	39.973	24.559	75.321	1.00	2.31
ATOM	507	OD2 ASP 1	65	39.216	25.329	73.383	1.00	2.31
ATOM	508	N GLN 1	66	34.923	23.176	74.437	1.00	4.28
ATOM	509	CA GLN 1	66	33.871	22.214	74.544	1.00	4.28
ATOM	510	C GLN 1	66	32.997	22.275	73.331	1.00	4.28
ATOM	511	O GLN 1	66	32.573	21.241	72.818	1.00	4.28
ATOM	512	CB GLN 1	66	33.060	22.315	75.850	1.00	4.28
ATOM	513	CG GLN 1	66	32.355	23.643	76.091	1.00	4.28
ATOM	514	CD GLN 1	66	31.667	23.538	77.446	1.00	4.28
ATOM	515	OE1 GLN 1	66	31.207	24.530	78.008	1.00	4.28
ATOM	516	NE2 GLN 1	66	31.603	22.296	77.997	1.00	4.28
ATOM	517	N MET 1	67	32.721	23.488	72.819	1.00	3.13
ATOM	518	CA MET 1	67	31.898	23.612	71.650	1.00	3.13
ATOM	519	C MET 1	67	32.571	22.973	70.468	1.00	3.13
ATOM	520	O MET 1	67	31.939	22.233	69.715	1.00	3.13
ATOM	521	CB MET 1	67	31.607	25.077	71.280	1.00	3.13
ATOM	522	CG MET 1	67	30.664	25.228	70.084	1.00	3.13
ATOM	523	SD MET 1	67	30.294	26.948	69.626	1.00	3.13
ATOM	524	CE MET 1	67	31.963	27.311	69.009	1.00	3.13
ATOM	525	N THR 1	68	33.886	23.223	70.288	1.00	5.42
ATOM	526	CA THR 1	68	34.602	22.693	69.158	1.00	5.42
ATOM	527	C THR 1	68	34.617	21.202	69.180	1.00	5.42
ATOM	528	O THR 1	68	34.468	20.547	68.153	1.00	5.42
ATOM	529	CB THR 1	68	36.045	23.110	69.088	1.00	5.42
ATOM	530	OG1 THR 1	68	36.730	22.735	70.274	1.00	5.42
ATOM	531	CG2 THR 1	68	36.138	24.620	68.855	1.00	5.42
ATOM	532	N LEU 1	69	34.805	20.625	70.369	1.00	4.63
ATOM	533	CA LEU 1	69	34.932	19.209	70.528	1.00	4.63
ATOM	534	C LEU 1	69	33.649	18.522	70.135	1.00	4.63
ATOM	535	O LEU 1	69	33.668	17.458	69.515	1.00	4.63
ATOM	536	CB LEU 1	69	35.364	18.942	71.982	1.00	4.63
ATOM	537	CG LEU 1	69	35.680	17.500	72.368	1.00	4.63
ATOM	538	CD1 LEU 1	69	36.393	17.456	73.731	1.00	4.63

109/208

ATOM	539	CD2 LEU 1	69	34.402	16.660	72.377	1.00	4.63
ATOM	540	N LEU 1	70	32.491	19.117	70.484	1.00	3.55
ATOM	541	CA LEU 1	70	31.209	18.564	70.139	1.00	3.55
ATOM	542	C LEU 1	70	31.023	18.656	68.654	1.00	3.55
ATOM	543	O LEU 1	70	30.531	17.729	68.011	1.00	3.55
ATOM	544	CB LEU 1	70	30.063	19.334	70.829	1.00	3.55
ATOM	545	CG LEU 1	70	28.646	18.719	70.748	1.00	3.55
ATOM	546	CD1 LEU 1	70	27.651	19.623	71.485	1.00	3.55
ATOM	547	CD2 LEU 1	70	28.175	18.417	69.314	1.00	3.55
ATOM	548	N GLN 1	71	31.417	19.794	68.065	1.00	3.95
ATOM	549	CA GLN 1	71	31.204	20.011	66.669	1.00	3.95
ATOM	550	C GLN 1	71	32.006	19.031	65.867	1.00	3.95
ATOM	551	O GLN 1	71	31.579	18.612	64.791	1.00	3.95
ATOM	552	CB GLN 1	71	31.568	21.451	66.279	1.00	3.95
ATOM	553	CG GLN 1	71	30.966	21.902	64.956	1.00	3.95
ATOM	554	CD GLN 1	71	30.911	23.421	65.006	1.00	3.95
ATOM	555	OE1 GLN 1	71	31.916	24.103	65.206	1.00	3.95
ATOM	556	NE2 GLN 1	71	29.677	23.971	64.852	1.00	3.95
ATOM	557	N TYR 1	72	33.225	18.690	66.340	1.00	4.09
ATOM	558	CA TYR 1	72	34.080	17.754	65.656	1.00	4.09
ATOM	559	C TYR 1	72	33.570	16.343	65.724	1.00	4.09
ATOM	560	O TYR 1	72	33.602	15.594	64.749	1.00	4.09
ATOM	561	CB TYR 1	72	35.523	17.725	66.214	1.00	4.09
ATOM	562	CG TYR 1	72	36.110	19.104	66.193	1.00	4.09
ATOM	563	CD1 TYR 1	72	36.146	19.840	65.034	1.00	4.09
ATOM	564	CD2 TYR 1	72	36.860	19.556	67.257	1.00	4.09
ATOM	565	CE1 TYR 1	72	36.796	21.046	64.957	1.00	4.09
ATOM	566	CE2 TYR 1	72	37.529	20.759	67.192	1.00	4.09
ATOM	567	CZ TYR 1	72	37.486	21.514	66.044	1.00	4.09
ATOM	568	OH TYR 1	72	38.169	22.746	65.962	1.00	4.09
ATOM	569	N SER 1	73	33.144	15.947	66.930	1.00	1.90
ATOM	570	CA SER 1	73	32.739	14.620	67.315	1.00	1.90
ATOM	571	C SER 1	73	31.344	14.111	67.096	1.00	1.90
ATOM	572	O SER 1	73	31.133	12.901	67.159	1.00	1.90
ATOM	573	CB SER 1	73	33.055	14.338	68.794	1.00	1.90
ATOM	574	OG SER 1	73	32.243	15.147	69.631	1.00	1.90
ATOM	575	N TRP 1	74	30.348	14.988	66.875	1.00	1.47
ATOM	576	CA TRP 1	74	28.973	14.557	66.922	1.00	1.47
ATOM	577	C TRP 1	74	28.678	13.369	66.047	1.00	1.47
ATOM	578	O TRP 1	74	28.008	12.436	66.488	1.00	1.47
ATOM	579	CB TRP 1	74	27.998	15.678	66.520	1.00	1.47
ATOM	580	CG TRP 1	74	28.085	16.095	65.072	1.00	1.47
ATOM	581	CD1 TRP 1	74	28.924	16.982	64.464	1.00	1.47
ATOM	582	CD2 TRP 1	74	27.155	15.661	64.068	1.00	1.47
ATOM	583	NE1 TRP 1	74	28.588	17.113	63.137	1.00	1.47
ATOM	584	CE2 TRP 1	74	27.496	16.310	62.882	1.00	1.47
ATOM	585	CE3 TRP 1	74	26.098	14.800	64.134	1.00	1.47
ATOM	586	CZ2 TRP 1	74	26.783	16.102	61.737	1.00	1.47
ATOM	587	CZ3 TRP 1	74	25.382	14.591	62.977	1.00	1.47

110/208

ATOM	588	CH2 TRP	1	74	25.719	15.230	61.801	1.00	1.47
ATOM	589	N MET	1	75	29.179	13.348	64.799	1.00	8.65
ATOM	590	CA MET	1	75	28.914	12.245	63.909	1.00	8.65
ATOM	591	C MET	1	75	29.449	10.969	64.476	1.00	8.65
ATOM	592	O MET	1	75	28.795	9.928	64.442	1.00	8.65
ATOM	593	CB MET	1	75	29.654	12.355	62.562	1.00	8.65
ATOM	594	CG MET	1	75	29.113	13.388	61.582	1.00	8.65
ATOM	595	SD MET	1	75	27.569	12.911	60.754	1.00	8.65
ATOM	596	CE MET	1	75	27.660	14.291	59.579	1.00	8.65
ATOM	597	N PHE	1	76	30.680	11.037	65.002	1.00	6.18
ATOM	598	CA PHE	1	76	31.420	9.914	65.494	1.00	6.18
ATOM	599	C PHE	1	76	30.657	9.318	66.645	1.00	6.18
ATOM	600	O PHE	1	76	30.457	8.106	66.712	1.00	6.18
ATOM	601	CB PHE	1	76	32.777	10.430	66.015	1.00	6.18
ATOM	602	CG PHE	1	76	33.873	9.429	65.892	1.00	6.18
ATOM	603	CD1 PHE	1	76	34.022	8.395	66.780	1.00	6.18
ATOM	604	CD2 PHE	1	76	34.898	9.693	65.013	1.00	6.18
ATOM	605	CE1 PHE	1	76	35.157	7.616	66.761	1.00	6.18
ATOM	606	CE2 PHE	1	76	36.038	8.926	64.993	1.00	6.18
ATOM	607	CZ PHE	1	76	36.175	7.890	65.882	1.00	6.18
ATOM	608	N LEU	1	77	30.188	10.172	67.576	1.00	0.90
ATOM	609	CA LEU	1	77	29.472	9.716	68.736	1.00	0.90
ATOM	610	C LEU	1	77	28.177	9.076	68.347	1.00	0.90
ATOM	611	O LEU	1	77	27.792	8.046	68.902	1.00	0.90
ATOM	612	CB LEU	1	77	29.124	10.853	69.712	1.00	0.90
ATOM	613	CG LEU	1	77	30.343	11.484	70.408	1.00	0.90
ATOM	614	CD1 LEU	1	77	29.906	12.608	71.360	1.00	0.90
ATOM	615	CD2 LEU	1	77	31.201	10.420	71.112	1.00	0.90
ATOM	616	N MET	1	78	27.461	9.682	67.385	1.00	3.39
ATOM	617	CA MET	1	78	26.169	9.206	66.980	1.00	3.39
ATOM	618	C MET	1	78	26.256	7.850	66.344	1.00	3.39
ATOM	619	O MET	1	78	25.462	6.962	66.650	1.00	3.39
ATOM	620	CB MET	1	78	25.521	10.127	65.931	1.00	3.39
ATOM	621	CG MET	1	78	25.394	11.589	66.368	1.00	3.39
ATOM	622	SD MET	1	78	24.325	11.892	67.804	1.00	3.39
ATOM	623	CE MET	1	78	24.452	13.702	67.722	1.00	3.39
ATOM	624	N ALA	1	79	27.226	7.663	65.428	1.00	1.42
ATOM	625	CA ALA	1	79	27.373	6.418	64.725	1.00	1.42
ATOM	626	C ALA	1	79	27.784	5.339	65.684	1.00	1.42
ATOM	627	O ALA	1	79	27.378	4.183	65.554	1.00	1.42
ATOM	628	CB ALA	1	79	28.436	6.484	63.613	1.00	1.42
ATOM	629	N PHE	1	80	28.630	5.701	66.665	1.00	4.87
ATOM	630	CA PHE	1	80	29.131	4.776	67.643	1.00	4.87
ATOM	631	C PHE	1	80	27.961	4.289	68.446	1.00	4.87
ATOM	632	O PHE	1	80	27.832	3.097	68.731	1.00	4.87
ATOM	633	CB PHE	1	80	30.128	5.481	68.591	1.00	4.87
ATOM	634	CG PHE	1	80	31.005	4.494	69.285	1.00	4.87
ATOM	635	CD1 PHE	1	80	30.669	3.929	70.489	1.00	4.87
ATOM	636	CD2 PHE	1	80	32.240	4.204	68.766	1.00	4.87



111/208

ATOM	637	CE1 PHE	1	80	31.541	3.085	71.140	1.00	4.87
ATOM	638	CE2 PHE	1	80	33.110	3.357	69.408	1.00	4.87
ATOM	639	CZ PHE	1	80	32.767	2.789	70.604	1.00	4.87
ATOM	640	N ALA	1	81	27.061	5.221	68.816	1.00	0.63
ATOM	641	CA ALA	1	81	25.899	4.891	69.593	1.00	0.63
ATOM	642	C ALA	1	81	25.013	3.977	68.800	1.00	0.63
ATOM	643	O ALA	1	81	24.439	3.030	69.337	1.00	0.63
ATOM	644	CB ALA	1	81	25.065	6.128	69.966	1.00	0.63
ATOM	645	N LEU	1	82	24.889	4.247	67.486	1.00	4.41
ATOM	646	CA LEU	1	82	24.068	3.458	66.610	1.00	4.41
ATOM	647	C LEU	1	82	24.616	2.070	66.661	1.00	4.41
ATOM	648	O LEU	1	82	23.873	1.092	66.763	1.00	4.41
ATOM	649	CB LEU	1	82	24.174	3.949	65.147	1.00	4.41
ATOM	650	CG LEU	1	82	23.343	3.203	64.072	1.00	4.41
ATOM	651	CD1 LEU	1	82	23.781	1.752	63.854	1.00	4.41
ATOM	652	CD2 LEU	1	82	21.840	3.322	64.339	1.00	4.41
ATOM	653	N GLY	1	83	25.956	1.959	66.610	1.00	0.71
ATOM	654	CA GLY	1	83	26.551	0.656	66.624	1.00	0.71
ATOM	655	C GLY	1	83	26.209	-0.053	67.891	1.00	0.71
ATOM	656	O GLY	1	83	25.846	-1.230	67.875	1.00	0.71
ATOM	657	N TRP	1	84	26.312	0.647	69.036	1.00	5.43
ATOM	658	CA TRP	1	84	26.070	-0.084	70.238	1.00	5.43
ATOM	659	C TRP	1	84	24.644	-0.492	70.371	1.00	5.43
ATOM	660	O TRP	1	84	24.377	-1.570	70.885	1.00	5.43
ATOM	661	CB TRP	1	84	26.530	0.587	71.534	1.00	5.43
ATOM	662	CG TRP	1	84	26.714	-0.487	72.576	1.00	5.43
ATOM	663	CD1 TRP	1	84	27.620	-1.503	72.549	1.00	5.43
ATOM	664	CD2 TRP	1	84	25.993	-0.628	73.804	1.00	5.43
ATOM	665	NE1 TRP	1	84	27.490	-2.282	73.667	1.00	5.43
ATOM	666	CE2 TRP	1	84	26.489	-1.762	74.449	1.00	5.43
ATOM	667	CE3 TRP	1	84	25.004	0.121	74.350	1.00	5.43
ATOM	668	CZ2 TRP	1	84	25.993	-2.175	75.648	1.00	5.43
ATOM	669	CZ3 TRP	1	84	24.521	-0.293	75.566	1.00	5.43
ATOM	670	CH2 TRP	1	84	24.986	-1.424	76.197	1.00	5.43
ATOM	671	N ARG	1	85	23.680	0.347	69.945	1.00	7.10
ATOM	672	CA ARG	1	85	22.302	-0.062	70.044	1.00	7.10
ATOM	673	C ARG	1	85	21.943	-1.219	69.137	1.00	7.10
ATOM	674	O ARG	1	85	21.117	-2.053	69.506	1.00	7.10
ATOM	675	CB ARG	1	85	21.334	1.119	69.846	1.00	7.10
ATOM	676	CG ARG	1	85	21.549	1.909	68.557	1.00	7.10
ATOM	677	CD ARG	1	85	20.961	3.320	68.634	1.00	7.10
ATOM	678	NE ARG	1	85	21.336	4.032	67.380	1.00	7.10
ATOM	679	CZ ARG	1	85	21.148	5.380	67.289	1.00	7.10
ATOM	680	NH1 ARG	1	85	20.612	6.062	68.343	1.00	7.10
ATOM	681	NH2 ARG	1	85	21.491	6.044	66.147	1.00	7.10
ATOM	682	N SER	1	86	22.527	-1.297	67.919	1.00	4.93
ATOM	683	CA SER	1	86	22.239	-2.347	66.954	1.00	4.93
ATOM	684	C SER	1	86	22.731	-3.699	67.418	1.00	4.93
ATOM	685	O SER	1	86	22.118	-4.736	67.201	1.00	4.93

112/208

ATOM	686	CB	SER	1	86	22.780	-2.038	65.543	1.00	4.93
ATOM	687	OG	SER	1	86	24.177	-1.799	65.572	1.00	4.93
ATOM	688	N	TYR	1	87	23.740	-3.599	68.271	1.00	5.71
ATOM	689	CA	TYR	1	87	24.722	-4.268	69.053	1.00	5.71
ATOM	690	C	TYR	1	87	23.797	-4.370	70.201	1.00	5.71
ATOM	691	O	TYR	1	87	22.949	-3.542	70.391	1.00	5.71
ATOM	692	CB	TYR	1	87	25.916	-3.424	69.523	1.00	5.71
ATOM	693	CG	TYR	1	87	26.607	-4.240	70.565	1.00	5.71
ATOM	694	CD1	TYR	1	87	27.507	-5.222	70.215	1.00	5.71
ATOM	695	CD2	TYR	1	87	26.295	-4.074	71.895	1.00	5.71
ATOM	696	CE1	TYR	1	87	28.105	-6.003	71.177	1.00	5.71
ATOM	697	CE2	TYR	1	87	26.876	-4.864	72.860	1.00	5.71
ATOM	698	CZ	TYR	1	87	27.793	-5.821	72.503	1.00	5.71
ATOM	699	OH	TYR	1	87	28.403	-6.622	73.491	1.00	5.71
ATOM	700	N	ARG	1	88	23.651	-5.475	70.882	1.00	11.72
ATOM	701	CA	ARG	1	88	22.545	-6.028	71.589	1.00	11.72
ATOM	702	C	ARG	1	88	21.089	-5.674	71.453	1.00	11.72
ATOM	703	O	ARG	1	88	20.291	-6.542	71.804	1.00	11.72
ATOM	704	CB	ARG	1	88	22.920	-5.950	73.084	1.00	11.72
ATOM	705	CG	ARG	1	88	21.818	-5.469	74.021	1.00	11.72
ATOM	706	CD	ARG	1	88	22.173	-5.588	75.505	1.00	11.72
ATOM	707	NE	ARG	1	88	23.480	-4.919	75.748	1.00	11.72
ATOM	708	CZ	ARG	1	88	24.070	-5.048	76.973	1.00	11.72
ATOM	709	NH1	ARG	1	88	23.453	-5.777	77.949	1.00	11.72
ATOM	710	NH2	ARG	1	88	25.274	-4.457	77.226	1.00	11.72
ATOM	711	N	GLN	1	89	20.621	-4.489	71.058	1.00	4.60
ATOM	712	CA	GLN	1	89	19.203	-4.505	70.793	1.00	4.60
ATOM	713	C	GLN	1	89	18.855	-5.524	69.711	1.00	4.60
ATOM	714	O	GLN	1	89	17.867	-6.245	69.854	1.00	4.60
ATOM	715	CB	GLN	1	89	18.679	-3.141	70.312	1.00	4.60
ATOM	716	CG	GLN	1	89	18.840	-2.013	71.336	1.00	4.60
ATOM	717	CD	GLN	1	89	17.787	-2.169	72.427	1.00	4.60
ATOM	718	OE1	GLN	1	89	17.342	-1.180	73.008	1.00	4.60
ATOM	719	NE2	GLN	1	89	17.378	-3.431	72.722	1.00	4.60
ATOM	720	N	SER	1	90	19.645	-5.639	68.610	1.00	2.81
ATOM	721	CA	SER	1	90	19.280	-6.556	67.551	1.00	2.81
ATOM	722	C	SER	1	90	20.424	-7.420	67.087	1.00	2.81
ATOM	723	O	SER	1	90	20.424	-7.886	65.947	1.00	2.81
ATOM	724	CB	SER	1	90	18.752	-5.830	66.302	1.00	2.81
ATOM	725	OG	SER	1	90	19.785	-5.049	65.718	1.00	2.81
ATOM	726	N	SER	1	91	21.429	-7.669	67.951	1.00	3.74
ATOM	727	CA	SER	1	91	22.507	-8.560	67.595	1.00	3.74
ATOM	728	C	SER	1	91	23.278	-8.110	66.390	1.00	3.74
ATOM	729	O	SER	1	91	23.876	-8.922	65.683	1.00	3.74
ATOM	730	CB	SER	1	91	22.028	-9.999	67.336	1.00	3.74
ATOM	731	OG	SER	1	91	21.476	-10.550	68.522	1.00	3.74
ATOM	732	N	ALA	1	92	23.308	-6.789	66.147	1.00	1.75
ATOM	733	CA	ALA	1	92	24.041	-6.197	65.060	1.00	1.75
ATOM	734	C	ALA	1	92	23.484	-6.566	63.718	1.00	1.75

113/208

ATOM	735	O	ALA	1	92	24.097	-6.277	62.691	1.00	1.75
ATOM	736	CB	ALA	1	92	25.531	-6.580	65.070	1.00	1.75
ATOM	737	N	ASN	1	93	22.299	-7.204	63.703	1.00	1.99
ATOM	738	CA	ASN	1	93	21.631	-7.643	62.505	1.00	1.99
ATOM	739	C	ASN	1	93	21.009	-6.533	61.709	1.00	1.99
ATOM	740	O	ASN	1	93	20.905	-6.627	60.485	1.00	1.99
ATOM	741	CB	ASN	1	93	20.515	-8.661	62.794	1.00	1.99
ATOM	742	CG	ASN	1	93	21.168	-9.945	63.287	1.00	1.99
ATOM	743	OD1	ASN	1	93	20.496	-10.843	63.792	1.00	1.99
ATOM	744	ND2	ASN	1	93	22.517	-10.033	63.144	1.00	1.99
ATOM	745	N	LEU	1	94	20.521	-5.479	62.390	1.00	0.96
ATOM	746	CA	LEU	1	94	19.880	-4.388	61.710	1.00	0.96
ATOM	747	C	LEU	1	94	20.429	-3.134	62.313	1.00	0.96
ATOM	748	O	LEU	1	94	21.133	-3.185	63.320	1.00	0.96
ATOM	749	CB	LEU	1	94	18.355	-4.359	61.899	1.00	0.96
ATOM	750	CG	LEU	1	94	17.639	-5.581	61.295	1.00	0.96
ATOM	751	CD1	LEU	1	94	16.120	-5.501	61.511	1.00	0.96
ATOM	752	CD2	LEU	1	94	18.023	-5.780	59.820	1.00	0.96
ATOM	753	N	LEU	1	95	20.147	-1.967	61.693	1.00	3.62
ATOM	754	CA	LEU	1	95	20.646	-0.735	62.243	1.00	3.62
ATOM	755	C	LEU	1	95	19.565	-0.166	63.102	1.00	3.62
ATOM	756	O	LEU	1	95	18.527	0.265	62.603	1.00	3.62
ATOM	757	CB	LEU	1	95	20.954	0.327	61.172	1.00	3.62
ATOM	758	CG	LEU	1	95	22.168	0.034	60.269	1.00	3.62
ATOM	759	CD1	LEU	1	95	23.490	0.393	60.953	1.00	3.62
ATOM	760	CD2	LEU	1	95	22.162	-1.420	59.788	1.00	3.62
ATOM	761	N	CYS	1	96	19.764	-0.139	64.433	1.00	4.51
ATOM	762	CA	CYS	1	96	18.683	0.408	65.190	1.00	4.51
ATOM	763	C	CYS	1	96	18.976	1.828	65.556	1.00	4.51
ATOM	764	O	CYS	1	96	19.596	2.141	66.571	1.00	4.51
ATOM	765	CB	CYS	1	96	18.219	-0.417	66.413	1.00	4.51
ATOM	766	SG	CYS	1	96	19.291	-0.380	67.867	1.00	4.51
ATOM	767	N	PHE	1	97	18.527	2.749	64.686	1.00	0.88
ATOM	768	CA	PHE	1	97	18.736	4.145	64.915	1.00	0.88
ATOM	769	C	PHE	1	97	17.946	4.578	66.113	1.00	0.88
ATOM	770	O	PHE	1	97	18.428	5.352	66.938	1.00	0.88
ATOM	771	CB	PHE	1	97	18.340	5.023	63.714	1.00	0.88
ATOM	772	CG	PHE	1	97	19.305	4.748	62.607	1.00	0.88
ATOM	773	CD1	PHE	1	97	19.077	3.728	61.712	1.00	0.88
ATOM	774	CD2	PHE	1	97	20.453	5.497	62.477	1.00	0.88
ATOM	775	CE1	PHE	1	97	19.966	3.474	60.695	1.00	0.88
ATOM	776	CE2	PHE	1	97	21.350	5.242	61.466	1.00	0.88
ATOM	777	CZ	PHE	1	97	21.104	4.233	60.568	1.00	0.88
ATOM	778	N	ALA	1	98	16.694	4.094	66.232	1.00	0.99
ATOM	779	CA	ALA	1	98	15.862	4.421	67.357	1.00	0.99
ATOM	780	C	ALA	1	98	14.863	3.309	67.454	1.00	0.99
ATOM	781	O	ALA	1	98	14.773	2.480	66.551	1.00	0.99
ATOM	782	CB	ALA	1	98	15.081	5.735	67.181	1.00	0.99
ATOM	783	N	PRO	1	99	14.113	3.239	68.522	1.00	1.69

114/208

ATOM	784	CA	PRO	1	99	13.143	2.183	68.629	1.00	1.69
ATOM	785	C	PRO	1	99	12.092	2.311	67.572	1.00	1.69
ATOM	786	O	PRO	1	99	11.548	1.296	67.140	1.00	1.69
ATOM	787	CB	PRO	1	99	12.632	2.242	70.066	1.00	1.69
ATOM	788	CG	PRO	1	99	13.837	2.804	70.847	1.00	1.69
ATOM	789	CD	PRO	1	99	14.591	3.674	69.824	1.00	1.69
ATOM	790	N	ASP	1	100	11.757	3.555	67.192	1.00	1.75
ATOM	791	CA	ASP	1	100	10.802	3.836	66.160	1.00	1.75
ATOM	792	C	ASP	1	100	11.387	3.687	64.790	1.00	1.75
ATOM	793	O	ASP	1	100	10.637	3.615	63.820	1.00	1.75
ATOM	794	CB	ASP	1	100	10.150	5.228	66.271	1.00	1.75
ATOM	795	CG	ASP	1	100	11.209	6.304	66.121	1.00	1.75
ATOM	796	OD1	ASP	1	100	12.253	6.218	66.820	1.00	1.75
ATOM	797	OD2	ASP	1	100	10.985	7.228	65.295	1.00	1.75
ATOM	798	N	LEU	1	101	12.732	3.746	64.662	1.00	1.92
ATOM	799	CA	LEU	1	101	13.358	3.662	63.368	1.00	1.92
ATOM	800	C	LEU	1	101	14.440	2.619	63.354	1.00	1.92
ATOM	801	O	LEU	1	101	15.581	2.886	63.732	1.00	1.92
ATOM	802	CB	LEU	1	101	13.994	5.010	62.969	1.00	1.92
ATOM	803	CG	LEU	1	101	14.853	5.009	61.688	1.00	1.92
ATOM	804	CD1	LEU	1	101	14.049	4.622	60.438	1.00	1.92
ATOM	805	CD2	LEU	1	101	15.571	6.358	61.523	1.00	1.92
ATOM	806	N	ILE	1	102	14.113	1.399	62.879	1.00	3.39
ATOM	807	CA	ILE	1	102	15.094	0.355	62.783	1.00	3.39
ATOM	808	C	ILE	1	102	15.201	0.038	61.323	1.00	3.39
ATOM	809	O	ILE	1	102	14.186	-0.155	60.656	1.00	3.39
ATOM	810	CB	ILE	1	102	14.709	-0.926	63.477	1.00	3.39
ATOM	811	CG1	ILE	1	102	14.529	-0.719	64.991	1.00	3.39
ATOM	812	CG2	ILE	1	102	15.774	-1.979	63.134	1.00	3.39
ATOM	813	CD1	ILE	1	102	13.243	0.008	65.374	1.00	3.39
ATOM	814	N	ILE	1	103	16.436	-0.029	60.779	1.00	4.51
ATOM	815	CA	ILE	1	103	16.560	-0.283	59.374	1.00	4.51
ATOM	816	C	ILE	1	103	17.129	-1.634	59.093	1.00	4.51
ATOM	817	O	ILE	1	103	18.055	-2.108	59.748	1.00	4.51
ATOM	818	CB	ILE	1	103	17.407	0.716	58.636	1.00	4.51
ATOM	819	CG1	ILE	1	103	18.857	0.673	59.134	1.00	4.51
ATOM	820	CG2	ILE	1	103	16.744	2.096	58.778	1.00	4.51
ATOM	821	CD1	ILE	1	103	19.831	1.443	58.243	1.00	4.51
ATOM	822	N	ASN	1	104	16.548	-2.265	58.062	1.00	4.77
ATOM	823	CA	ASN	1	104	16.843	-3.577	57.583	1.00	4.77
ATOM	824	C	ASN	1	104	17.201	-3.356	56.144	1.00	4.77
ATOM	825	O	ASN	1	104	16.881	-2.306	55.592	1.00	4.77
ATOM	826	CB	ASN	1	104	15.562	-4.421	57.659	1.00	4.77
ATOM	827	CG	ASN	1	104	15.739	-5.726	56.930	1.00	4.77
ATOM	828	OD1	ASN	1	104	15.674	-5.768	55.703	1.00	4.77
ATOM	829	ND2	ASN	1	104	15.945	-6.822	57.703	1.00	4.77
ATOM	830	N	GLU	1	105	17.855	-4.338	55.489	1.00	6.85
ATOM	831	CA	GLU	1	105	18.307	-4.145	54.137	1.00	6.85
ATOM	832	C	GLU	1	105	17.168	-3.846	53.217	1.00	6.85

SUBSTITUTE SHEET (RULE 26)

115/208

ATOM	833	O	GLU 1 105	17.317	-3.074	52.273	1.00	6.85
ATOM	834	CB	GLU 1 105	19.109	-5.319	53.541	1.00	6.85
ATOM	835	CG	GLU 1 105	18.321	-6.616	53.372	1.00	6.85
ATOM	836	CD	GLU 1 105	18.211	-7.282	54.738	1.00	6.85
ATOM	837	OE1	GLU 1 105	18.830	-6.762	55.704	1.00	6.85
ATOM	838	OE2	GLU 1 105	17.507	-8.323	54.832	1.00	6.85
ATOM	839	N	GLN 1 106	15.987	-4.435	53.465	1.00	3.68
ATOM	840	CA	GLN 1 106	14.888	-4.206	52.576	1.00	3.68
ATOM	841	C	GLN 1 106	14.583	-2.741	52.519	1.00	3.68
ATOM	842	O	GLN 1 106	14.276	-2.208	51.456	1.00	3.68
ATOM	843	CB	GLN 1 106	13.615	-4.962	52.999	1.00	3.68
ATOM	844	CG	GLN 1 106	13.061	-4.546	54.363	1.00	3.68
ATOM	845	CD	GLN 1 106	11.816	-5.379	54.632	1.00	3.68
ATOM	846	OE1	GLN 1 106	11.323	-6.085	53.753	1.00	3.68
ATOM	847	NE2	GLN 1 106	11.294	-5.300	55.885	1.00	3.68
ATOM	848	N	ARG 1 107	14.651	-2.051	53.670	1.00	6.71
ATOM	849	CA	ARG 1 107	14.369	-0.647	53.733	1.00	6.71
ATOM	850	C	ARG 1 107	15.397	0.257	53.114	1.00	6.71
ATOM	851	O	ARG 1 107	15.080	1.401	52.795	1.00	6.71
ATOM	852	CB	ARG 1 107	13.931	-0.177	55.129	1.00	6.71
ATOM	853	CG	ARG 1 107	14.838	-0.579	56.282	1.00	6.71
ATOM	854	CD	ARG 1 107	14.205	-0.220	57.627	1.00	6.71
ATOM	855	NE	ARG 1 107	12.773	-0.633	57.597	1.00	6.71
ATOM	856	CZ	ARG 1 107	11.801	0.262	57.252	1.00	6.71
ATOM	857	NH1	ARG 1 107	10.493	-0.128	57.243	1.00	6.71
ATOM	858	NH2	ARG 1 107	12.132	1.546	56.924	1.00	6.71
ATOM	859	N	MET 1 108	16.669	-0.171	52.971	1.00	7.61
ATOM	860	CA	MET 1 108	17.574	0.739	52.321	1.00	7.61
ATOM	861	C	MET 1 108	17.626	0.489	50.841	1.00	7.61
ATOM	862	O	MET 1 108	18.500	-0.215	50.338	1.00	7.61
ATOM	863	CB	MET 1 108	19.014	0.755	52.878	1.00	7.61
ATOM	864	CG	MET 1 108	19.680	-0.604	53.099	1.00	7.61
ATOM	865	SD	MET 1 108	19.434	-1.350	54.736	1.00	7.61
ATOM	866	CE	MET 1 108	20.502	-0.222	55.677	1.00	7.61
ATOM	867	N	THR 1 109	16.653	1.068	50.106	1.00	5.21
ATOM	868	CA	THR 1 109	16.574	0.937	48.678	1.00	5.21
ATOM	869	C	THR 1 109	17.645	1.713	47.974	1.00	5.21
ATOM	870	O	THR 1 109	18.330	1.188	47.097	1.00	5.21
ATOM	871	CB	THR 1 109	15.263	1.422	48.132	1.00	5.21
ATOM	872	OG1	THR 1 109	15.110	2.810	48.390	1.00	5.21
ATOM	873	CG2	THR 1 109	14.127	0.631	48.802	1.00	5.21
ATOM	874	N	LEU 1 110	17.835	2.987	48.372	1.00	6.15
ATOM	875	CA	LEU 1 110	18.754	3.865	47.704	1.00	6.15
ATOM	876	C	LEU 1 110	20.118	3.254	47.804	1.00	6.15
ATOM	877	O	LEU 1 110	20.606	2.945	48.890	1.00	6.15
ATOM	878	CB	LEU 1 110	18.716	5.280	48.323	1.00	6.15
ATOM	879	CG	LEU 1 110	19.494	6.380	47.577	1.00	6.15
ATOM	880	CD1	LEU 1 110	21.006	6.245	47.767	1.00	6.15
ATOM	881	CD2	LEU 1 110	19.081	6.446	46.098	1.00	6.15

116/208

ATOM	882	N	PRO	1	111	20.729	3.040	46.668	1.00	5.04
ATOM	883	CA	PRO	1	111	22.012	2.390	46.633	1.00	5.04
ATOM	884	C	PRO	1	111	23.112	3.146	47.305	1.00	5.04
ATOM	885	O	PRO	1	111	23.973	2.516	47.918	1.00	5.04
ATOM	886	CB	PRO	1	111	22.274	2.068	45.164	1.00	5.04
ATOM	887	CG	PRO	1	111	20.859	1.908	44.576	1.00	5.04
ATOM	888	CD	PRO	1	111	19.973	2.815	45.447	1.00	5.04
ATOM	889	N	CYS	1	112	23.121	4.484	47.192	1.00	0.66
ATOM	890	CA	CYS	1	112	24.142	5.271	47.817	1.00	0.66
ATOM	891	C	CYS	1	112	23.989	5.156	49.297	1.00	0.66
ATOM	892	O	CYS	1	112	24.966	4.996	50.028	1.00	0.66
ATOM	893	CB	CYS	1	112	24.043	6.765	47.466	1.00	0.66
ATOM	894	SG	CYS	1	112	24.332	7.087	45.700	1.00	0.66
ATOM	895	N	MET	1	113	22.733	5.242	49.769	1.00	3.18
ATOM	896	CA	MET	1	113	22.433	5.193	51.167	1.00	3.18
ATOM	897	C	MET	1	113	22.748	3.849	51.740	1.00	3.18
ATOM	898	O	MET	1	113	23.314	3.754	52.829	1.00	3.18
ATOM	899	CB	MET	1	113	20.949	5.478	51.457	1.00	3.18
ATOM	900	CG	MET	1	113	20.599	5.458	52.946	1.00	3.18
ATOM	901	SD	MET	1	113	18.849	5.795	53.310	1.00	3.18
ATOM	902	CE	MET	1	113	18.935	7.557	52.885	1.00	3.18
ATOM	903	N	TYR	1	114	22.391	2.751	51.045	1.00	7.80
ATOM	904	CA	TYR	1	114	22.695	1.531	51.725	1.00	7.80
ATOM	905	C	TYR	1	114	24.163	1.278	51.734	1.00	7.80
ATOM	906	O	TYR	1	114	24.678	0.611	52.629	1.00	7.80
ATOM	907	CB	TYR	1	114	21.893	0.261	51.375	1.00	7.80
ATOM	908	CG	TYR	1	114	22.306	-0.518	50.184	1.00	7.80
ATOM	909	CD1	TYR	1	114	21.577	-0.433	49.024	1.00	7.80
ATOM	910	CD2	TYR	1	114	23.153	-1.587	50.369	1.00	7.80
ATOM	911	CE1	TYR	1	114	21.679	-1.424	48.077	1.00	7.80
ATOM	912	CE2	TYR	1	114	23.282	-2.562	49.412	1.00	7.80
ATOM	913	CZ	TYR	1	114	22.517	-2.496	48.275	1.00	7.80
ATOM	914	OH	TYR	1	114	22.572	-3.541	47.330	1.00	7.80
ATOM	915	N	ASP	1	115	24.887	1.809	50.735	1.00	4.14
ATOM	916	CA	ASP	1	115	26.308	1.631	50.732	1.00	4.14
ATOM	917	C	ASP	1	115	26.814	2.261	51.992	1.00	4.14
ATOM	918	O	ASP	1	115	27.707	1.733	52.653	1.00	4.14
ATOM	919	CB	ASP	1	115	26.993	2.331	49.545	1.00	4.14
ATOM	920	CG	ASP	1	115	28.461	1.929	49.534	1.00	4.14
ATOM	921	OD1	ASP	1	115	29.180	2.348	48.588	1.00	4.14
ATOM	922	OD2	ASP	1	115	28.882	1.193	50.466	1.00	4.14
ATOM	923	N	GLN	1	116	26.238	3.421	52.360	1.00	2.66
ATOM	924	CA	GLN	1	116	26.637	4.121	53.546	1.00	2.66
ATOM	925	C	GLN	1	116	26.311	3.286	54.750	1.00	2.66
ATOM	926	O	GLN	1	116	27.085	3.237	55.705	1.00	2.66
ATOM	927	CB	GLN	1	116	25.934	5.487	53.680	1.00	2.66
ATOM	928	CG	GLN	1	116	26.323	6.282	54.928	1.00	2.66
ATOM	929	CD	GLN	1	116	25.405	5.871	56.069	1.00	2.66
ATOM	930	OE1	GLN	1	116	25.635	6.236	57.220	1.00	2.66

117/208

ATOM	931	NE2 GLN	1 116	24.330	5.104	55.745	1.00	2.66
ATOM	932	N CYS	1 117	25.151	2.600	54.731	1.00	0.90
ATOM	933	CA CYS	1 117	24.729	1.792	55.843	1.00	0.90
ATOM	934	C CYS	1 117	25.679	0.662	56.073	1.00	0.90
ATOM	935	O CYS	1 117	25.979	0.312	57.214	1.00	0.90
ATOM	936	CB CYS	1 117	23.328	1.185	55.654	1.00	0.90
ATOM	937	SG CYS	1 117	22.022	2.449	55.682	1.00	0.90
ATOM	938	N LYS	1 118	26.185	0.063	54.982	1.00	4.62
ATOM	939	CA LYS	1 118	27.083	-1.046	55.097	1.00	4.62
ATOM	940	C LYS	1 118	28.284	-0.562	55.835	1.00	4.62
ATOM	941	O LYS	1 118	28.868	-1.283	56.642	1.00	4.62
ATOM	942	CB LYS	1 118	27.556	-1.566	53.728	1.00	4.62
ATOM	943	CG LYS	1 118	28.508	-2.760	53.815	1.00	4.62
ATOM	944	CD LYS	1 118	28.748	-3.443	52.467	1.00	4.62
ATOM	945	CE LYS	1 118	27.506	-4.136	51.901	1.00	4.62
ATOM	946	NZ LYS	1 118	27.821	-4.746	50.590	1.00	4.62
ATOM	947	N HIS	1 119	28.687	0.687	55.551	1.00	4.28
ATOM	948	CA HIS	1 119	29.831	1.283	56.167	1.00	4.28
ATOM	949	C HIS	1 119	29.583	1.420	57.639	1.00	4.28
ATOM	950	O HIS	1 119	30.446	1.079	58.448	1.00	4.28
ATOM	951	CB HIS	1 119	30.108	2.673	55.569	1.00	4.28
ATOM	952	CG HIS	1 119	31.467	3.225	55.867	1.00	4.28
ATOM	953	ND1 HIS	1 119	32.643	2.608	55.502	1.00	4.28
ATOM	954	CD2 HIS	1 119	31.824	4.440	56.364	1.00	4.28
ATOM	955	CE1 HIS	1 119	33.647	3.468	55.803	1.00	4.28
ATOM	956	NE2 HIS	1 119	33.197	4.595	56.325	1.00	4.28
ATOM	957	N MET	1 120	28.391	1.912	58.045	1.00	7.65
ATOM	958	CA MET	1 120	28.194	2.013	59.463	1.00	7.65
ATOM	959	C MET	1 120	28.060	0.670	60.109	1.00	7.65
ATOM	960	O MET	1 120	28.397	0.505	61.278	1.00	7.65
ATOM	961	CB MET	1 120	27.096	2.955	60.020	1.00	7.65
ATOM	962	CG MET	1 120	25.636	2.694	59.675	1.00	7.65
ATOM	963	SD MET	1 120	25.017	3.639	58.262	1.00	7.65
ATOM	964	CE MET	1 120	23.295	3.110	58.489	1.00	7.65
ATOM	965	N LEU	1 121	27.592	-0.333	59.348	1.00	7.58
ATOM	966	CA LEU	1 121	27.347	-1.667	59.827	1.00	7.58
ATOM	967	C LEU	1 121	28.611	-2.254	60.386	1.00	7.58
ATOM	968	O LEU	1 121	28.573	-3.128	61.250	1.00	7.58
ATOM	969	CB LEU	1 121	26.815	-2.579	58.700	1.00	7.58
ATOM	970	CG LEU	1 121	26.520	-4.042	59.093	1.00	7.58
ATOM	971	CD1 LEU	1 121	27.803	-4.867	59.280	1.00	7.58
ATOM	972	CD2 LEU	1 121	25.582	-4.108	60.309	1.00	7.58
ATOM	973	N TYR	1 122	29.777	-1.785	59.913	1.00	0.69
ATOM	974	CA TYR	1 122	31.023	-2.339	60.358	1.00	0.69
ATOM	975	C TYR	1 122	31.168	-2.246	61.850	1.00	0.69
ATOM	976	O TYR	1 122	31.742	-3.141	62.468	1.00	0.69
ATOM	977	CB TYR	1 122	32.243	-1.652	59.722	1.00	0.69
ATOM	978	CG TYR	1 122	32.225	-1.982	58.269	1.00	0.69
ATOM	979	CD1 TYR	1 122	32.714	-3.189	57.823	1.00	0.69

118/208

ATOM	980	CD2 TYR 1 122	31.727	-1.087	57.351	1.00	0.69
ATOM	981	CE1 TYR 1 122	32.699	-3.501	56.484	1.00	0.69
ATOM	982	CE2 TYR 1 122	31.710	-1.392	56.010	1.00	0.69
ATOM	983	CZ TYR 1 122	32.195	-2.602	55.575	1.00	0.69
ATOM	984	OH TYR 1 122	32.176	-2.919	54.201	1.00	0.69
ATOM	985	N VAL 1 123	30.676	-1.160	62.477	1.00	3.47
ATOM	986	CA VAL 1 123	30.837	-1.018	63.900	1.00	3.47
ATOM	987	C VAL 1 123	30.149	-2.098	64.691	1.00	3.47
ATOM	988	O VAL 1 123	30.777	-2.759	65.515	1.00	3.47
ATOM	989	CB VAL 1 123	30.340	0.309	64.404	1.00	3.47
ATOM	990	CG1 VAL 1 123	31.208	1.416	63.783	1.00	3.47
ATOM	991	CG2 VAL 1 123	28.844	0.445	64.075	1.00	3.47
ATOM	992	N SER 1 124	28.854	-2.356	64.434	1.00	0.91
ATOM	993	CA SER 1 124	28.133	-3.337	65.201	1.00	0.91
ATOM	994	C SER 1 124	28.804	-4.660	65.027	1.00	0.91
ATOM	995	O SER 1 124	28.880	-5.461	65.958	1.00	0.91
ATOM	996	CB SER 1 124	26.677	-3.501	64.737	1.00	0.91
ATOM	997	OG SER 1 124	26.642	-4.017	63.415	1.00	0.91
ATOM	998	N SER 1 125	29.311	-4.921	63.812	1.00	3.19
ATOM	999	CA SER 1 125	29.950	-6.171	63.518	1.00	3.19
ATOM	1000	C SER 1 125	31.149	-6.353	64.395	1.00	3.19
ATOM	1001	O SER 1 125	31.382	-7.440	64.920	1.00	3.19
ATOM	1002	CB SER 1 125	30.432	-6.263	62.061	1.00	3.19
ATOM	1003	OG SER 1 125	29.321	-6.233	61.178	1.00	3.19
ATOM	1004	N GLU 1 126	31.954	-5.289	64.570	1.00	3.11
ATOM	1005	CA GLU 1 126	33.127	-5.381	65.392	1.00	3.11
ATOM	1006	C GLU 1 126	32.716	-5.589	66.813	1.00	3.11
ATOM	1007	O GLU 1 126	33.373	-6.320	67.553	1.00	3.11
ATOM	1008	CB GLU 1 126	34.006	-4.119	65.341	1.00	3.11
ATOM	1009	CG GLU 1 126	34.707	-3.940	63.994	1.00	3.11
ATOM	1010	CD GLU 1 126	35.640	-5.129	63.802	1.00	3.11
ATOM	1011	OE1 GLU 1 126	35.848	-5.885	64.788	1.00	3.11
ATOM	1012	OE2 GLU 1 126	36.156	-5.297	62.665	1.00	3.11
ATOM	1013	N LEU 1 127	31.616	-4.934	67.235	1.00	3.70
ATOM	1014	CA LEU 1 127	31.166	-5.078	68.587	1.00	3.70
ATOM	1015	C LEU 1 127	30.795	-6.497	68.858	1.00	3.70
ATOM	1016	O LEU 1 127	31.127	-7.029	69.915	1.00	3.70
ATOM	1017	CB LEU 1 127	29.962	-4.186	68.948	1.00	3.70
ATOM	1018	CG LEU 1 127	30.327	-2.724	69.279	1.00	3.70
ATOM	1019	CD1 LEU 1 127	31.093	-2.640	70.609	1.00	3.70
ATOM	1020	CD2 LEU 1 127	31.083	-2.036	68.136	1.00	3.70
ATOM	1021	N HIS 1 128	30.097	-7.152	67.913	1.00	3.09
ATOM	1022	CA HIS 1 128	29.723	-8.521	68.119	1.00	3.09
ATOM	1023	C HIS 1 128	30.943	-9.388	68.199	1.00	3.09
ATOM	1024	O HIS 1 128	31.056	-10.246	69.074	1.00	3.09
ATOM	1025	CB HIS 1 128	28.840	-9.071	66.986	1.00	3.09
ATOM	1026	CG HIS 1 128	28.369	-10.473	67.237	1.00	3.09
ATOM	1027	ND1 HIS 1 128	27.246	-10.789	67.969	1.00	3.09
ATOM	1028	CD2 HIS 1 128	28.898	-11.662	66.836	1.00	3.09



119/208

ATOM 1029	CE1 HIS 1 128	27.151 -12.143 67.975 1.00 3.09
ATOM 1030	NE2 HIS 1 128	28.131 -12.716 67.300 1.00 3.09
ATOM 1031	N ARG 1 129	31.906 -9.176 67.286 1.00 3.04
ATOM 1032	CA ARG 1 129	33.067 -10.023 67.264 1.00 3.04
ATOM 1033	C ARG 1 129	33.843 -9.890 68.540 1.00 3.04
ATOM 1034	O ARG 1 129	34.161 -10.882 69.195 1.00 3.04
ATOM 1035	CB ARG 1 129	34.023 -9.667 66.112 1.00 3.04
ATOM 1036	CG ARG 1 129	35.201 -10.632 65.965 1.00 3.04
ATOM 1037	CD ARG 1 129	36.150 -10.270 64.821 1.00 3.04
ATOM 1038	NE ARG 1 129	37.233 -11.294 64.801 1.00 3.04
ATOM 1039	CZ ARG 1 129	38.348 -11.132 65.570 1.00 3.04
ATOM 1040	NH1 ARG 1 129	39.335 -12.075 65.547 1.00 3.04
ATOM 1041	NH2 ARG 1 129	38.478 -10.029 66.365 1.00 3.04
ATOM 1042	N LEU 1 130	34.148 -8.638 68.924 1.00 1.27
ATOM 1043	CA LEU 1 130	34.912 -8.315 70.098 1.00 1.27
ATOM 1044	C LEU 1 130	34.140 -8.585 71.349 1.00 1.27
ATOM 1045	O LEU 1 130	34.726 -8.841 72.402 1.00 1.27
ATOM 1046	CB LEU 1 130	35.349 -6.840 70.154 1.00 1.27
ATOM 1047	CG LEU 1 130	36.357 -6.449 69.058 1.00 1.27
ATOM 1048	CD1 LEU 1 130	36.756 -4.967 69.166 1.00 1.27
ATOM 1049	CD2 LEU 1 130	37.568 -7.395 69.056 1.00 1.27
ATOM 1050	N GLN 1 131	32.800 -8.512 71.280 1.00 3.66
ATOM 1051	CA GLN 1 131	32.028 -8.721 72.465 1.00 3.66
ATOM 1052	C GLN 1 131	32.351 -7.633 73.444 1.00 3.66
ATOM 1053	O GLN 1 131	32.692 -7.886 74.598 1.00 3.66
ATOM 1054	CB GLN 1 131	32.317 -10.086 73.107 1.00 3.66
ATOM 1055	CG GLN 1 131	31.424 -10.404 74.298 1.00 3.66
ATOM 1056	CD GLN 1 131	31.824 -11.775 74.824 1.00 3.66
ATOM 1057	OE1 GLN 1 131	32.705 -12.433 74.273 1.00 3.66
ATOM 1058	NE2 GLN 1 131	31.157 -12.222 75.922 1.00 3.66
ATOM 1059	N VAL 1 132	32.242 -6.372 72.973 1.00 1.28
ATOM 1060	CA VAL 1 132	32.502 -5.198 73.762 1.00 1.28
ATOM 1061	C VAL 1 132	31.545 -5.125 74.907 1.00 1.28
ATOM 1062	O VAL 1 132	30.359 -5.417 74.766 1.00 1.28
ATOM 1063	CB VAL 1 132	32.332 -3.926 72.979 1.00 1.28
ATOM 1064	CG1 VAL 1 132	32.333 -2.726 73.943 1.00 1.28
ATOM 1065	CG2 VAL 1 132	33.438 -3.871 71.912 1.00 1.28
ATOM 1066	N SER 1 133	32.065 -4.719 76.083 1.00 3.60
ATOM 1067	CA SER 1 133	31.288 -4.615 77.284 1.00 3.60
ATOM 1068	C SER 1 133	30.703 -3.246 77.382 1.00 3.60
ATOM 1069	O SER 1 133	31.171 -2.297 76.754 1.00 3.60
ATOM 1070	CB SER 1 133	32.135 -4.715 78.559 1.00 3.60
ATOM 1071	OG SER 1 133	33.062 -5.779 78.468 1.00 3.60
ATOM 1072	N TYR 1 134	29.669 -3.112 78.231 1.00 3.87
ATOM 1073	CA TYR 1 134	29.038 -1.843 78.423 1.00 3.87
ATOM 1074	C TYR 1 134	30.064 -0.924 79.016 1.00 3.87
ATOM 1075	O TYR 1 134	30.149 0.244 78.643 1.00 3.87
ATOM 1076	CB TYR 1 134	27.849 -1.915 79.396 1.00 3.87
ATOM 1077	CG TYR 1 134	27.208 -0.571 79.429 1.00 3.87

SUBSTITUTE SHEET (RULE 26)

120/208

ATOM	1078	CD1 TYR 1 134	27.732	0.446	80.191	1.00	3.87
ATOM	1079	CD2 TYR 1 134	26.052	-0.339	78.721	1.00	3.87
ATOM	1080	CE1 TYR 1 134	27.105	1.667	80.243	1.00	3.87
ATOM	1081	CE2 TYR 1 134	25.432	0.887	78.753	1.00	3.87
ATOM	1082	CZ TYR 1 134	25.961	1.896	79.520	1.00	3.87
ATOM	1083	OH TYR 1 134	25.333	3.159	79.566	1.00	3.87
ATOM	1084	N GLU 1 135	30.883	-1.434	79.957	1.00	5.78
ATOM	1085	CA GLU 1 135	31.859	-0.601	80.599	1.00	5.78
ATOM	1086	C GLU 1 135	32.885	-0.112	79.621	1.00	5.78
ATOM	1087	O GLU 1 135	33.347	1.025	79.700	1.00	5.78
ATOM	1088	CB GLU 1 135	32.589	-1.300	81.763	1.00	5.78
ATOM	1089	CG GLU 1 135	33.356	-2.570	81.385	1.00	5.78
ATOM	1090	CD GLU 1 135	32.391	-3.750	81.391	1.00	5.78
ATOM	1091	OE1 GLU 1 135	31.166	-3.532	81.582	1.00	5.78
ATOM	1092	OE2 GLU 1 135	32.875	-4.896	81.197	1.00	5.78
ATOM	1093	N GLU 1 136	33.286	-0.980	78.682	1.00	3.49
ATOM	1094	CA GLU 1 136	34.276	-0.676	77.692	1.00	3.49
ATOM	1095	C GLU 1 136	33.736	0.366	76.745	1.00	3.49
ATOM	1096	O GLU 1 136	34.420	1.323	76.380	1.00	3.49
ATOM	1097	CB GLU 1 136	34.580	-1.976	76.932	1.00	3.49
ATOM	1098	CG GLU 1 136	36.007	-2.148	76.438	1.00	3.49
ATOM	1099	CD GLU 1 136	36.196	-3.653	76.286	1.00	3.49
ATOM	1100	OE1 GLU 1 136	35.422	-4.270	75.507	1.00	3.49
ATOM	1101	OE2 GLU 1 136	37.102	-4.210	76.963	1.00	3.49
ATOM	1102	N TYR 1 137	32.459	0.208	76.351	1.00	1.07
ATOM	1103	CA TYR 1 137	31.774	1.072	75.425	1.00	1.07
ATOM	1104	C TYR 1 137	31.710	2.476	75.955	1.00	1.07
ATOM	1105	O TYR 1 137	31.964	3.439	75.229	1.00	1.07
ATOM	1106	CB TYR 1 137	30.329	0.568	75.207	1.00	1.07
ATOM	1107	CG TYR 1 137	29.561	1.518	74.358	1.00	1.07
ATOM	1108	CD1 TYR 1 137	29.695	1.512	72.990	1.00	1.07
ATOM	1109	CD2 TYR 1 137	28.597	2.314	74.931	1.00	1.07
ATOM	1110	CE1 TYR 1 137	28.904	2.320	72.209	1.00	1.07
ATOM	1111	CE2 TYR 1 137	27.814	3.134	74.155	1.00	1.07
ATOM	1112	CZ TYR 1 137	27.974	3.144	72.791	1.00	1.07
ATOM	1113	OH TYR 1 137	27.165	3.979	71.990	1.00	1.07
ATOM	1114	N LEU 1 138	31.391	2.624	77.254	1.00	1.14
ATOM	1115	CA LEU 1 138	31.235	3.929	77.836	1.00	1.14
ATOM	1116	C LEU 1 138	32.502	4.725	77.769	1.00	1.14
ATOM	1117	O LEU 1 138	32.474	5.919	77.474	1.00	1.14
ATOM	1118	CB LEU 1 138	30.862	3.910	79.328	1.00	1.14
ATOM	1119	CG LEU 1 138	29.457	3.381	79.651	1.00	1.14
ATOM	1120	CD1 LEU 1 138	29.143	3.587	81.143	1.00	1.14
ATOM	1121	CD2 LEU 1 138	28.393	3.991	78.723	1.00	1.14
ATOM	1122	N CYS 1 139	33.645	4.088	78.084	1.00	1.03
ATOM	1123	CA CYS 1 139	34.923	4.743	78.092	1.00	1.03
ATOM	1124	C CYS 1 139	35.315	5.115	76.696	1.00	1.03
ATOM	1125	O CYS 1 139	35.836	6.200	76.445	1.00	1.03
ATOM	1126	CB CYS 1 139	36.025	3.817	78.627	1.00	1.03

121/208

ATOM 1127 SG CYS 1 139	35.597	3.111	80.246	1.00	1.03
ATOM 1128 N MET 1 140	35.070	4.209	75.735	1.00	1.00
ATOM 1129 CA MET 1 140	35.468	4.495	74.387	1.00	1.00
ATOM 1130 C MET 1 140	34.720	5.683	73.874	1.00	1.00
ATOM 1131 O MET 1 140	35.275	6.502	73.150	1.00	1.00
ATOM 1132 CB MET 1 140	35.236	3.338	73.402	1.00	1.00
ATOM 1133 CG MET 1 140	36.172	2.154	73.642	1.00	1.00
ATOM 1134 SD MET 1 140	35.935	0.762	72.499	1.00	1.00
ATOM 1135 CE MET 1 140	36.614	1.644	71.064	1.00	1.00
ATOM 1136 N LYS 1 141	33.440	5.821	74.255	1.00	8.36
ATOM 1137 CA LYS 1 141	32.600	6.896	73.798	1.00	8.36
ATOM 1138 C LYS 1 141	33.239	8.207	74.142	1.00	8.36
ATOM 1139 O LYS 1 141	33.265	9.126	73.324	1.00	8.36
ATOM 1140 CB LYS 1 141	31.266	6.892	74.563	1.00	8.36
ATOM 1141 CG LYS 1 141	30.210	5.896	74.094	1.00	8.36
ATOM 1142 CD LYS 1 141	29.337	6.420	72.957	1.00	8.36
ATOM 1143 CE LYS 1 141	28.021	7.015	73.475	1.00	8.36
ATOM 1144 NZ LYS 1 141	28.282	7.977	74.575	1.00	8.36
ATOM 1145 N THR 1 142	33.757	8.333	75.380	1.00	4.68
ATOM 1146 CA THR 1 142	34.342	9.572	75.806	1.00	4.68
ATOM 1147 C THR 1 142	35.582	9.858	75.018	1.00	4.68
ATOM 1148 O THR 1 142	35.838	10.999	74.639	1.00	4.68
ATOM 1149 CB THR 1 142	34.699	9.614	77.266	1.00	4.68
ATOM 1150 OG1 THR 1 142	34.996	10.947	77.652	1.00	4.68
ATOM 1151 CG2 THR 1 142	35.920	8.717	77.518	1.00	4.68
ATOM 1152 N LEU 1 143	36.380	8.813	74.733	1.00	1.09
ATOM 1153 CA LEU 1 143	37.596	8.982	73.995	1.00	1.09
ATOM 1154 C LEU 1 143	37.268	9.518	72.634	1.00	1.09
ATOM 1155 O LEU 1 143	38.052	10.264	72.047	1.00	1.09
ATOM 1156 CB LEU 1 143	38.401	7.680	73.834	1.00	1.09
ATOM 1157 CG LEU 1 143	39.033	7.181	75.150	1.00	1.09
ATOM 1158 CD1 LEU 1 143	39.825	5.882	74.932	1.00	1.09
ATOM 1159 CD2 LEU 1 143	39.883	8.279	75.812	1.00	1.09
ATOM 1160 N LEU 1 144	36.107	9.127	72.080	1.00	4.43
ATOM 1161 CA LEU 1 144	35.669	9.620	70.802	1.00	4.43
ATOM 1162 C LEU 1 144	35.448	11.105	70.850	1.00	4.43
ATOM 1163 O LEU 1 144	35.804	11.807	69.905	1.00	4.43
ATOM 1164 CB LEU 1 144	34.345	8.988	70.331	1.00	4.43
ATOM 1165 CG LEU 1 144	34.469	7.624	69.623	1.00	4.43
ATOM 1166 CD1 LEU 1 144	35.238	6.580	70.428	1.00	4.43
ATOM 1167 CD2 LEU 1 144	33.083	7.095	69.244	1.00	4.43
ATOM 1168 N LEU 1 145	34.859	11.633	71.947	1.00	7.68
ATOM 1169 CA LEU 1 145	34.649	13.060	72.019	1.00	7.68
ATOM 1170 C LEU 1 145	35.968	13.755	71.901	1.00	7.68
ATOM 1171 O LEU 1 145	36.092	14.810	71.286	1.00	7.68
ATOM 1172 CB LEU 1 145	34.168	13.631	73.373	1.00	7.68
ATOM 1173 CG LEU 1 145	32.665	13.714	73.671	1.00	7.68
ATOM 1174 CD1 LEU 1 145	31.946	14.615	72.655	1.00	7.68
ATOM 1175 CD2 LEU 1 145	32.028	12.343	73.869	1.00	7.68

122/208

ATOM 1176 N LEU 1 146	36.964	13.187	72.583	1.00	2.09
ATOM 1177 CA LEU 1 146	38.313	13.644	72.745	1.00	2.09
ATOM 1178 C LEU 1 146	39.224	13.344	71.590	1.00	2.09
ATOM 1179 O LEU 1 146	40.428	13.562	71.694	1.00	2.09
ATOM 1180 CB LEU 1 146	38.957	13.045	74.006	1.00	2.09
ATOM 1181 CG LEU 1 146	38.174	13.370	75.294	1.00	2.09
ATOM 1182 CD1 LEU 1 146	38.845	12.755	76.532	1.00	2.09
ATOM 1183 CD2 LEU 1 146	37.921	14.879	75.436	1.00	2.09
ATOM 1184 N SER 1 147	38.702	12.687	70.541	1.00	1.91
ATOM 1185 CA SER 1 147	39.438	12.173	69.420	1.00	1.91
ATOM 1186 C SER 1 147	40.101	13.132	68.468	1.00	1.91
ATOM 1187 O SER 1 147	41.080	12.752	67.830	1.00	1.91
ATOM 1188 CB SER 1 147	38.556	11.238	68.576	1.00	1.91
ATOM 1189 OG SER 1 147	39.322	10.657	67.535	1.00	1.91
ATOM 1190 N SER 1 148	39.570	14.355	68.262	1.00	1.23
ATOM 1191 CA SER 1 148	40.202	15.238	67.315	1.00	1.23
ATOM 1192 C SER 1 148	40.247	16.631	67.864	1.00	1.23
ATOM 1193 O SER 1 148	39.362	17.032	68.619	1.00	1.23
ATOM 1194 CB SER 1 148	39.460	15.310	65.971	1.00	1.23
ATOM 1195 OG SER 1 148	39.439	14.026	65.364	1.00	1.23
ATOM 1196 N VAL 1 149	41.297	17.412	67.515	1.00	2.96
ATOM 1197 CA VAL 1 149	41.290	18.766	67.989	1.00	2.96
ATOM 1198 C VAL 1 149	41.865	19.635	66.902	1.00	2.96
ATOM 1199 O VAL 1 149	42.328	19.128	65.881	1.00	2.96
ATOM 1200 CB VAL 1 149	42.008	18.984	69.297	1.00	2.96
ATOM 1201 CG1 VAL 1 149	43.323	19.756	69.103	1.00	2.96
ATOM 1202 CG2 VAL 1 149	40.995	19.585	70.278	1.00	2.96
ATOM 1203 N PRO 1 150	41.840	20.932	67.070	1.00	1.47
ATOM 1204 CA PRO 1 150	42.293	21.827	66.038	1.00	1.47
ATOM 1205 C PRO 1 150	43.760	21.693	65.799	1.00	1.47
ATOM 1206 O PRO 1 150	44.470	21.226	66.687	1.00	1.47
ATOM 1207 CB PRO 1 150	41.879	23.223	66.496	1.00	1.47
ATOM 1208 CG PRO 1 150	40.654	22.967	67.394	1.00	1.47
ATOM 1209 CD PRO 1 150	40.887	21.561	67.969	1.00	1.47
ATOM 1210 N LYS 1 151	44.233	22.091	64.601	1.00	7.70
ATOM 1211 CA LYS 1 151	45.627	21.985	64.285	1.00	7.70
ATOM 1212 C LYS 1 151	46.373	22.845	65.252	1.00	7.70
ATOM 1213 O LYS 1 151	47.477	22.508	65.674	1.00	7.70
ATOM 1214 CB LYS 1 151	45.969	22.422	62.847	1.00	7.70
ATOM 1215 CG LYS 1 151	45.445	23.804	62.455	1.00	7.70
ATOM 1216 CD LYS 1 151	43.917	23.896	62.448	1.00	7.70
ATOM 1217 CE LYS 1 151	43.378	25.217	61.895	1.00	7.70
ATOM 1218 NZ LYS 1 151	43.413	25.197	60.415	1.00	7.70
ATOM 1219 N ASP 1 152	45.768	23.990	65.613	1.00	4.33
ATOM 1220 CA ASP 1 152	46.301	24.933	66.553	1.00	4.33
ATOM 1221 C ASP 1 152	46.338	24.294	67.911	1.00	4.33
ATOM 1222 O ASP 1 152	47.229	24.555	68.719	1.00	4.33
ATOM 1223 CB ASP 1 152	45.407	26.180	66.648	1.00	4.33
ATOM 1224 CG ASP 1 152	46.062	27.198	67.562	1.00	4.33

123/208

ATOM	1225	OD1 ASP	1	152	47.234	26.977	67.967	1.00	4.33
ATOM	1226	OD2 ASP	1	152	45.394	28.222	67.868	1.00	4.33
ATOM	1227	N GLY	1	153	45.359	23.420	68.201	1.00	2.44
ATOM	1228	CA GLY	1	153	45.294	22.834	69.507	1.00	2.44
ATOM	1229	C GLY	1	153	44.183	23.547	70.208	1.00	2.44
ATOM	1230	O GLY	1	153	43.566	24.446	69.639	1.00	2.44
ATOM	1231	N LEU	1	154	43.904	23.152	71.467	1.00	1.42
ATOM	1232	CA LEU	1	154	42.822	23.715	72.225	1.00	1.42
ATOM	1233	C LEU	1	154	43.372	24.737	73.167	1.00	1.42
ATOM	1234	O LEU	1	154	44.554	24.721	73.504	1.00	1.42
ATOM	1235	CB LEU	1	154	42.091	22.689	73.118	1.00	1.42
ATOM	1236	CG LEU	1	154	41.267	21.609	72.388	1.00	1.42
ATOM	1237	CD1 LEU	1	154	40.595	20.649	73.387	1.00	1.42
ATOM	1238	CD2 LEU	1	154	40.227	22.221	71.435	1.00	1.42
ATOM	1239	N LYS	1	155	42.510	25.676	73.602	1.00	1.13
ATOM	1240	CA LYS	1	155	42.936	26.678	74.532	1.00	1.13
ATOM	1241	C LYS	1	155	43.307	25.989	75.804	1.00	1.13
ATOM	1242	O LYS	1	155	44.310	26.323	76.433	1.00	1.13
ATOM	1243	CB LYS	1	155	41.839	27.702	74.866	1.00	1.13
ATOM	1244	CG LYS	1	155	41.486	28.617	73.694	1.00	1.13
ATOM	1245	CD LYS	1	155	40.266	29.502	73.952	1.00	1.13
ATOM	1246	CE LYS	1	155	40.053	30.567	72.876	1.00	1.13
ATOM	1247	NZ LYS	1	155	38.923	31.447	73.249	1.00	1.13
ATOM	1248	N SER	1	156	42.498	24.996	76.214	1.00	4.74
ATOM	1249	CA SER	1	156	42.757	24.284	77.431	1.00	4.74
ATOM	1250	C SER	1	156	43.387	22.972	77.079	1.00	4.74
ATOM	1251	O SER	1	156	42.895	21.908	77.453	1.00	4.74
ATOM	1252	CB SER	1	156	41.469	24.009	78.225	1.00	4.74
ATOM	1253	OG SER	1	156	40.569	23.231	77.451	1.00	4.74
ATOM	1254	N GLN	1	157	44.525	23.021	76.362	1.00	1.05
ATOM	1255	CA GLN	1	157	45.170	21.820	75.920	1.00	1.05
ATOM	1256	C GLN	1	157	45.643	20.998	77.079	1.00	1.05
ATOM	1257	O GLN	1	157	45.504	19.776	77.075	1.00	1.05
ATOM	1258	CB GLN	1	157	46.381	22.086	75.010	1.00	1.05
ATOM	1259	CG GLN	1	157	46.956	20.810	74.392	1.00	1.05
ATOM	1260	CD GLN	1	157	45.943	20.286	73.381	1.00	1.05
ATOM	1261	OE1 GLN	1	157	45.030	21.000	72.969	1.00	1.05
ATOM	1262	NE2 GLN	1	157	46.106	19.000	72.967	1.00	1.05
ATOM	1263	N GLU	1	158	46.212	21.644	78.114	1.00	0.94
ATOM	1264	CA GLU	1	158	46.742	20.891	79.214	1.00	0.94
ATOM	1265	C GLU	1	158	45.659	20.120	79.899	1.00	0.94
ATOM	1266	O GLU	1	158	45.817	18.930	80.171	1.00	0.94
ATOM	1267	CB GLU	1	158	47.424	21.774	80.272	1.00	0.94
ATOM	1268	CG GLU	1	158	48.706	22.437	79.763	1.00	0.94
ATOM	1269	CD GLU	1	158	49.284	23.279	80.891	1.00	0.94
ATOM	1270	OE1 GLU	1	158	48.666	23.303	81.988	1.00	0.94
ATOM	1271	OE2 GLU	1	158	50.354	23.907	80.670	1.00	0.94
ATOM	1272	N LEU	1	159	44.516	20.771	80.183	1.00	6.51
ATOM	1273	CA LEU	1	159	43.458	20.081	80.860	1.00	6.51

124/208

ATOM	1274	C	LEU	1	159	42.923	19.004	79.972	1.00	6.51
ATOM	1275	O	LEU	1	159	42.515	17.943	80.440	1.00	6.51
ATOM	1276	CB	LEU	1	159	42.317	21.002	81.343	1.00	6.51
ATOM	1277	CG	LEU	1	159	41.671	21.902	80.276	1.00	6.51
ATOM	1278	CD1	LEU	1	159	40.863	21.092	79.254	1.00	6.51
ATOM	1279	CD2	LEU	1	159	40.842	23.018	80.932	1.00	6.51
ATOM	1280	N	PHE	1	160	42.914	19.254	78.652	1.00	0.70
ATOM	1281	CA	PHE	1	160	42.424	18.300	77.701	1.00	0.70
ATOM	1282	C	PHE	1	160	43.261	17.057	77.743	1.00	0.70
ATOM	1283	O	PHE	1	160	42.737	15.943	77.743	1.00	0.70
ATOM	1284	CB	PHE	1	160	42.463	18.878	76.274	1.00	0.70
ATOM	1285	CG	PHE	1	160	42.008	17.861	75.284	1.00	0.70
ATOM	1286	CD1	PHE	1	160	40.669	17.641	75.049	1.00	0.70
ATOM	1287	CD2	PHE	1	160	42.936	17.229	74.489	1.00	0.70
ATOM	1288	CE1	PHE	1	160	40.265	16.779	74.055	1.00	0.70
ATOM	1289	CE2	PHE	1	160	42.539	16.371	73.492	1.00	0.70
ATOM	1290	CZ	PHE	1	160	41.202	16.146	73.273	1.00	0.70
ATOM	1291	N	ASP	1	161	44.595	17.217	77.804	1.00	2.07
ATOM	1292	CA	ASP	1	161	45.471	16.080	77.802	1.00	2.07
ATOM	1293	C	ASP	1	161	45.219	15.249	79.018	1.00	2.07
ATOM	1294	O	ASP	1	161	45.138	14.024	78.939	1.00	2.07
ATOM	1295	CB	ASP	1	161	46.959	16.474	77.823	1.00	2.07
ATOM	1296	CG	ASP	1	161	47.307	17.100	76.480	1.00	2.07
ATOM	1297	OD1	ASP	1	161	48.432	17.656	76.361	1.00	2.07
ATOM	1298	OD2	ASP	1	161	46.453	17.035	75.556	1.00	2.07
ATOM	1299	N	GLU	1	162	45.075	15.901	80.185	1.00	4.44
ATOM	1300	CA	GLU	1	162	44.878	15.164	81.396	1.00	4.44
ATOM	1301	C	GLU	1	162	43.575	14.430	81.337	1.00	4.44
ATOM	1302	O	GLU	1	162	43.483	13.287	81.782	1.00	4.44
ATOM	1303	CB	GLU	1	162	44.905	16.049	82.658	1.00	4.44
ATOM	1304	CG	GLU	1	162	43.824	17.129	82.707	1.00	4.44
ATOM	1305	CD	GLU	1	162	44.022	17.927	83.987	1.00	4.44
ATOM	1306	OE1	GLU	1	162	43.156	18.792	84.287	1.00	4.44
ATOM	1307	OE2	GLU	1	162	45.045	17.685	84.682	1.00	4.44
ATOM	1308	N	ILE	1	163	42.528	15.062	80.774	1.00	0.97
ATOM	1309	CA	ILE	1	163	41.251	14.412	80.717	1.00	0.97
ATOM	1310	C	ILE	1	163	41.348	13.174	79.880	1.00	0.97
ATOM	1311	O	ILE	1	163	40.853	12.117	80.271	1.00	0.97
ATOM	1312	CB	ILE	1	163	40.184	15.272	80.104	1.00	0.97
ATOM	1313	CG1	ILE	1	163	39.978	16.548	80.936	1.00	0.97
ATOM	1314	CG2	ILE	1	163	38.913	14.418	79.955	1.00	0.97
ATOM	1315	CD1	ILE	1	163	39.125	17.603	80.233	1.00	0.97
ATOM	1316	N	ARG	1	164	42.018	13.266	78.714	1.00	5.11
ATOM	1317	CA	ARG	1	164	42.112	12.133	77.835	1.00	5.11
ATOM	1318	C	ARG	1	164	42.798	11.013	78.542	1.00	5.11
ATOM	1319	O	ARG	1	164	42.361	9.866	78.486	1.00	5.11
ATOM	1320	CB	ARG	1	164	42.978	12.373	76.588	1.00	5.11
ATOM	1321	CG	ARG	1	164	42.373	13.301	75.545	1.00	5.11
ATOM	1322	CD	ARG	1	164	43.195	13.347	74.256	1.00	5.11

125/208

ATOM	1323	NE ARG 1 164	42.787	12.183	73.419	1.00	5.11
ATOM	1324	CZ ARG 1 164	43.376	10.963	73.583	1.00	5.11
ATOM	1325	NH1 ARG 1 164	44.321	10.774	74.550	1.00	5.11
ATOM	1326	NH2 ARG 1 164	43.013	9.929	72.770	1.00	5.11
ATOM	1327	N MET 1 165	43.897	11.331	79.244	1.00	5.20
ATOM	1328	CA MET 1 165	44.683	10.329	79.900	1.00	5.20
ATOM	1329	C MET 1 165	43.852	9.624	80.923	1.00	5.20
ATOM	1330	O MET 1 165	43.925	8.404	81.056	1.00	5.20
ATOM	1331	CB MET 1 165	45.916	10.942	80.591	1.00	5.20
ATOM	1332	CG MET 1 165	46.814	9.941	81.318	1.00	5.20
ATOM	1333	SD MET 1 165	46.178	9.395	82.929	1.00	5.20
ATOM	1334	CE MET 1 165	47.681	8.484	83.384	1.00	5.20
ATOM	1335	N THR 1 166	43.020	10.377	81.665	1.00	1.86
ATOM	1336	CA THR 1 166	42.227	9.776	82.696	1.00	1.86
ATOM	1337	C THR 1 166	41.281	8.781	82.099	1.00	1.86
ATOM	1338	O THR 1 166	41.107	7.687	82.633	1.00	1.86
ATOM	1339	CB THR 1 166	41.409	10.777	83.454	1.00	1.86
ATOM	1340	OG1 THR 1 166	42.256	11.741	84.062	1.00	1.86
ATOM	1341	CG2 THR 1 166	40.597	10.034	84.528	1.00	1.86
ATOM	1342	N TYR 1 167	40.633	9.138	80.976	1.00	4.58
ATOM	1343	CA TYR 1 167	39.712	8.236	80.346	1.00	4.58
ATOM	1344	C TYR 1 167	40.375	7.041	79.745	1.00	4.58
ATOM	1345	O TYR 1 167	39.795	5.956	79.725	1.00	4.58
ATOM	1346	CB TYR 1 167	38.807	8.904	79.299	1.00	4.58
ATOM	1347	CG TYR 1 167	37.739	9.600	80.072	1.00	4.58
ATOM	1348	CD1 TYR 1 167	37.899	10.876	80.557	1.00	4.58
ATOM	1349	CD2 TYR 1 167	36.585	8.922	80.383	1.00	4.58
ATOM	1350	CE1 TYR 1 167	36.903	11.471	81.298	1.00	4.58
ATOM	1351	CE2 TYR 1 167	35.584	9.512	81.117	1.00	4.58
ATOM	1352	CZ TYR 1 167	35.741	10.796	81.571	1.00	4.58
ATOM	1353	OH TYR 1 167	34.717	11.422	82.312	1.00	4.58
ATOM	1354	N ILE 1 168	41.591	7.203	79.193	1.00	4.85
ATOM	1355	CA ILE 1 168	42.252	6.046	78.673	1.00	4.85
ATOM	1356	C ILE 1 168	42.607	5.114	79.792	1.00	4.85
ATOM	1357	O ILE 1 168	42.560	3.896	79.634	1.00	4.85
ATOM	1358	CB ILE 1 168	43.380	6.367	77.726	1.00	4.85
ATOM	1359	CG1 ILE 1 168	44.398	7.344	78.319	1.00	4.85
ATOM	1360	CG2 ILE 1 168	42.748	6.849	76.412	1.00	4.85
ATOM	1361	CD1 ILE 1 168	45.536	7.660	77.347	1.00	4.85
ATOM	1362	N LYS 1 169	42.939	5.668	80.973	1.00	6.27
ATOM	1363	CA LYS 1 169	43.238	4.856	82.121	1.00	6.27
ATOM	1364	C LYS 1 169	41.992	4.099	82.471	1.00	6.27
ATOM	1365	O LYS 1 169	42.035	2.915	82.795	1.00	6.27
ATOM	1366	CB LYS 1 169	43.582	5.704	83.355	1.00	6.27
ATOM	1367	CG LYS 1 169	44.715	6.703	83.123	1.00	6.27
ATOM	1368	CD LYS 1 169	46.071	6.077	82.805	1.00	6.27
ATOM	1369	CE LYS 1 169	46.877	5.725	84.055	1.00	6.27
ATOM	1370	NZ LYS 1 169	48.286	5.481	83.687	1.00	6.27
ATOM	1371	N GLU 1 170	40.842	4.792	82.393	1.00	3.71

126/208

ATOM	1372	CA	GLU 1 170	39.535	4.287	82.702	1.00	3.71
ATOM	1373	C	GLU 1 170	39.184	3.129	81.813	1.00	3.71
ATOM	1374	O	GLU 1 170	38.618	2.135	82.266	1.00	3.71
ATOM	1375	CB	GLU 1 170	38.514	5.426	82.519	1.00	3.71
ATOM	1376	CG	GLU 1 170	37.104	5.005	82.131	1.00	3.71
ATOM	1377	CD	GLU 1 170	36.480	4.192	83.241	1.00	3.71
ATOM	1378	OE1	GLU 1 170	37.231	3.606	84.064	1.00	3.71
ATOM	1379	OE2	GLU 1 170	35.223	4.142	83.261	1.00	3.71
ATOM	1380	N	LEU 1 171	39.525	3.226	80.517	1.00	0.72
ATOM	1381	CA	LEU 1 171	39.238	2.176	79.584	1.00	0.72
ATOM	1382	C	LEU 1 171	39.997	0.961	80.009	1.00	0.72
ATOM	1383	O	LEU 1 171	39.512	-0.164	79.893	1.00	0.72
ATOM	1384	CB	LEU 1 171	39.674	2.534	78.152	1.00	0.72
ATOM	1385	CG	LEU 1 171	39.381	1.437	77.112	1.00	0.72
ATOM	1386	CD1	LEU 1 171	37.873	1.178	76.984	1.00	0.72
ATOM	1387	CD2	LEU 1 171	40.040	1.764	75.760	1.00	0.72
ATOM	1388	N	GLY 1 172	41.229	1.159	80.511	1.00	0.34
ATOM	1389	CA	GLY 1 172	42.030	0.051	80.940	1.00	0.34
ATOM	1390	C	GLY 1 172	41.331	-0.658	82.061	1.00	0.34
ATOM	1391	O	GLY 1 172	41.312	-1.888	82.100	1.00	0.34
ATOM	1392	N	LYS 1 173	40.736	0.098	83.009	1.00	4.65
ATOM	1393	CA	LYS 1 173	40.076	-0.530	84.122	1.00	4.65
ATOM	1394	C	LYS 1 173	38.922	-1.329	83.607	1.00	4.65
ATOM	1395	O	LYS 1 173	38.646	-2.427	84.081	1.00	4.65
ATOM	1396	CB	LYS 1 173	39.408	0.418	85.140	1.00	4.65
ATOM	1397	CG	LYS 1 173	40.289	1.453	85.840	1.00	4.65
ATOM	1398	CD	LYS 1 173	40.465	2.734	85.030	1.00	4.65
ATOM	1399	CE	LYS 1 173	41.022	3.903	85.841	1.00	4.65
ATOM	1400	NZ	LYS 1 173	42.467	3.709	86.083	1.00	4.65
ATOM	1401	N	ALA 1 174	38.194	-0.786	82.618	1.00	0.62
ATOM	1402	CA	ALA 1 174	37.042	-1.476	82.119	1.00	0.62
ATOM	1403	C	ALA 1 174	37.494	-2.785	81.562	1.00	0.62
ATOM	1404	O	ALA 1 174	36.845	-3.812	81.751	1.00	0.62
ATOM	1405	CB	ALA 1 174	36.331	-0.715	80.988	1.00	0.62
ATOM	1406	N	ILE 1 175	38.640	-2.765	80.862	1.00	4.02
ATOM	1407	CA	ILE 1 175	39.217	-3.929	80.253	1.00	4.02
ATOM	1408	C	ILE 1 175	39.540	-4.928	81.321	1.00	4.02
ATOM	1409	O	ILE 1 175	39.264	-6.119	81.178	1.00	4.02
ATOM	1410	CB	ILE 1 175	40.539	-3.616	79.608	1.00	4.02
ATOM	1411	CG1	ILE 1 175	40.398	-2.574	78.486	1.00	4.02
ATOM	1412	CG2	ILE 1 175	41.172	-4.942	79.163	1.00	4.02
ATOM	1413	CD1	ILE 1 175	39.588	-3.060	77.292	1.00	4.02
ATOM	1414	N	VAL 1 176	40.121	-4.453	82.440	1.00	1.20
ATOM	1415	CA	VAL 1 176	40.587	-5.342	83.465	1.00	1.20
ATOM	1416	C	VAL 1 176	39.463	-6.067	84.123	1.00	1.20
ATOM	1417	O	VAL 1 176	39.662	-7.154	84.662	1.00	1.20
ATOM	1418	CB	VAL 1 176	41.426	-4.700	84.542	1.00	1.20
ATOM	1419	CG1	VAL 1 176	42.626	-4.010	83.872	1.00	1.20
ATOM	1420	CG2	VAL 1 176	40.566	-3.806	85.444	1.00	1.20

SUBSTITUTE SHEET (RULE 26)



127/208

ATOM	1421	N	LYS	1	177	38.252	-5.483	84.122	1.00	9.34
ATOM	1422	CA	LYS	1	177	37.173	-6.140	84.794	1.00	9.34
ATOM	1423	C	LYS	1	177	36.987	-7.509	84.215	1.00	9.34
ATOM	1424	O	LYS	1	177	36.793	-8.474	84.950	1.00	9.34
ATOM	1425	CB	LYS	1	177	35.843	-5.372	84.655	1.00	9.34
ATOM	1426	CG	LYS	1	177	34.706	-5.886	85.546	1.00	9.34
ATOM	1427	CD	LYS	1	177	34.225	-7.301	85.213	1.00	9.34
ATOM	1428	CE	LYS	1	177	33.356	-7.371	83.955	1.00	9.34
ATOM	1429	NZ	LYS	1	177	34.185	-7.132	82.752	1.00	9.34
ATOM	1430	N	ARG	1	178	36.949	-7.602	82.876	1.00	6.15
ATOM	1431	CA	ARG	1	178	36.803	-8.830	82.146	1.00	6.15
ATOM	1432	C	ARG	1	178	38.089	-9.552	81.835	1.00	6.15
ATOM	1433	O	ARG	1	178	38.151	-10.779	81.870	1.00	6.15
ATOM	1434	CB	ARG	1	178	36.100	-8.536	80.816	1.00	6.15
ATOM	1435	CG	ARG	1	178	35.172	-9.641	80.330	1.00	6.15
ATOM	1436	CD	ARG	1	178	33.960	-9.792	81.253	1.00	6.15
ATOM	1437	NE	ARG	1	178	32.797	-10.215	80.427	1.00	6.15
ATOM	1438	CZ	ARG	1	178	31.923	-9.270	79.973	1.00	6.15
ATOM	1439	NH1	ARG	1	178	32.113	-7.958	80.297	1.00	6.15
ATOM	1440	NH2	ARG	1	178	30.855	-9.632	79.205	1.00	6.15
ATOM	1441	N	GLU	1	179	39.160	-8.795	81.512	1.00	5.83
ATOM	1442	CA	GLU	1	179	40.337	-9.414	80.964	1.00	5.83
ATOM	1443	C	GLU	1	179	41.421	-9.588	81.984	1.00	5.83
ATOM	1444	O	GLU	1	179	42.183	-8.665	82.267	1.00	5.83
ATOM	1445	CB	GLU	1	179	40.893	-8.582	79.801	1.00	5.83
ATOM	1446	CG	GLU	1	179	41.573	-9.440	78.749	1.00	5.83
ATOM	1447	CD	GLU	1	179	40.468	-10.276	78.116	1.00	5.83
ATOM	1448	OE1	GLU	1	179	39.682	-9.709	77.312	1.00	5.83
ATOM	1449	OE2	GLU	1	179	40.386	-11.492	78.438	1.00	5.83
ATOM	1450	N	GLY	1	180	41.525	-10.812	82.540	1.00	1.02
ATOM	1451	CA	GLY	1	180	42.476	-11.112	83.571	1.00	1.02
ATOM	1452	C	GLY	1	180	43.910	-11.102	83.135	1.00	1.02
ATOM	1453	O	GLY	1	180	44.758	-10.507	83.798	1.00	1.02
ATOM	1454	N	ASN	1	181	44.232	-11.755	82.001	1.00	3.29
ATOM	1455	CA	ASN	1	181	45.613	-11.860	81.628	1.00	3.29
ATOM	1456	C	ASN	1	181	46.206	-10.515	81.364	1.00	3.29
ATOM	1457	O	ASN	1	181	45.548	-9.582	80.907	1.00	3.29
ATOM	1458	CB	ASN	1	181	45.873	-12.755	80.400	1.00	3.29
ATOM	1459	CG	ASN	1	181	47.344	-13.150	80.358	1.00	3.29
ATOM	1460	OD1	ASN	1	181	48.113	-12.886	81.281	1.00	3.29
ATOM	1461	ND2	ASN	1	181	47.751	-13.816	79.244	1.00	3.29
ATOM	1462	N	SER	1	182	47.498	-10.375	81.696	1.00	0.74
ATOM	1463	CA	SER	1	182	48.172	-9.145	81.442	1.00	0.74
ATOM	1464	C	SER	1	182	48.248	-8.998	79.961	1.00	0.74
ATOM	1465	O	SER	1	182	48.082	-7.904	79.426	1.00	0.74
ATOM	1466	CB	SER	1	182	49.610	-9.127	81.988	1.00	0.74
ATOM	1467	OG	SER	1	182	50.400	-10.094	81.312	1.00	0.74
ATOM	1468	N	SER	1	183	48.541	-10.113	79.266	1.00	3.77
ATOM	1469	CA	SER	1	183	48.669	-10.105	77.840	1.00	3.77

128/208

ATOM	1470	C	SER 1 183	47.372	-9.935	77.115	1.00	3.77
ATOM	1471	O	SER 1 183	47.274	-9.086	76.229	1.00	3.77
ATOM	1472	CB	SER 1 183	49.314	-11.393	77.299	1.00	3.77
ATOM	1473	OG	SER 1 183	50.645	-11.510	77.779	1.00	3.77
ATOM	1474	N	GLN 1 184	46.325	-10.719	77.460	1.00	7.63
ATOM	1475	CA	GLN 1 184	45.186	-10.561	76.607	1.00	7.63
ATOM	1476	C	GLN 1 184	44.550	-9.246	76.903	1.00	7.63
ATOM	1477	O	GLN 1 184	43.887	-8.663	76.050	1.00	7.63
ATOM	1478	CB	GLN 1 184	44.127	-11.695	76.545	1.00	7.63
ATOM	1479	CG	GLN 1 184	42.965	-11.733	77.535	1.00	7.63
ATOM	1480	CD	GLN 1 184	43.429	-11.922	78.952	1.00	7.63
ATOM	1481	OE1	GLN 1 184	43.982	-10.984	79.514	1.00	7.63
ATOM	1482	NE2	GLN 1 184	43.165	-13.116	79.548	1.00	7.63
ATOM	1483	N	ASN 1 185	44.715	-8.751	78.144	1.00	3.79
ATOM	1484	CA	ASN 1 185	44.194	-7.463	78.495	1.00	3.79
ATOM	1485	C	ASN 1 185	44.890	-6.451	77.637	1.00	3.79
ATOM	1486	O	ASN 1 185	44.265	-5.531	77.111	1.00	3.79
ATOM	1487	CB	ASN 1 185	44.483	-7.108	79.967	1.00	3.79
ATOM	1488	CG	ASN 1 185	43.716	-5.849	80.347	1.00	3.79
ATOM	1489	OD1	ASN 1 185	42.795	-5.901	81.160	1.00	3.79
ATOM	1490	ND2	ASN 1 185	44.101	-4.687	79.754	1.00	3.79
ATOM	1491	N	TRP 1 186	46.220	-6.603	77.477	1.00	3.97
ATOM	1492	CA	TRP 1 186	46.982	-5.673	76.695	1.00	3.97
ATOM	1493	C	TRP 1 186	46.541	-5.785	75.275	1.00	3.97
ATOM	1494	O	TRP 1 186	46.382	-4.785	74.577	1.00	3.97
ATOM	1495	CB	TRP 1 186	48.496	-5.939	76.727	1.00	3.97
ATOM	1496	CG	TRP 1 186	49.305	-4.839	76.079	1.00	3.97
ATOM	1497	CD1	TRP 1 186	49.978	-3.811	76.672	1.00	3.97
ATOM	1498	CD2	TRP 1 186	49.426	-4.640	74.662	1.00	3.97
ATOM	1499	NE1	TRP 1 186	50.528	-2.994	75.713	1.00	3.97
ATOM	1500	CE2	TRP 1 186	50.192	-3.489	74.471	1.00	3.97
ATOM	1501	CE3	TRP 1 186	48.934	-5.351	73.605	1.00	3.97
ATOM	1502	CZ2	TRP 1 186	50.480	-3.032	73.217	1.00	3.97
ATOM	1503	CZ3	TRP 1 186	49.225	-4.887	72.341	1.00	3.97
ATOM	1504	CH2	TRP 1 186	49.983	-3.750	72.151	1.00	3.97
ATOM	1505	N	GLN 1 187	46.325	-7.028	74.815	1.00	0.67
ATOM	1506	CA	GLN 1 187	45.915	-7.248	73.464	1.00	0.67
ATOM	1507	C	GLN 1 187	44.575	-6.618	73.279	1.00	0.67
ATOM	1508	O	GLN 1 187	44.315	-6.017	72.237	1.00	0.67
ATOM	1509	CB	GLN 1 187	45.782	-8.742	73.124	1.00	0.67
ATOM	1510	CG	GLN 1 187	47.108	-9.501	73.209	1.00	0.67
ATOM	1511	CD	GLN 1 187	46.844	-10.957	72.853	1.00	0.67
ATOM	1512	OE1	GLN 1 187	45.725	-11.334	72.508	1.00	0.67
ATOM	1513	NE2	GLN 1 187	47.905	-11.804	72.942	1.00	0.67
ATOM	1514	N	ARG 1 188	43.674	-6.734	74.277	1.00	7.01
ATOM	1515	CA	ARG 1 188	42.393	-6.152	74.025	1.00	7.01
ATOM	1516	C	ARG 1 188	42.471	-4.662	73.982	1.00	7.01
ATOM	1517	O	ARG 1 188	41.707	-4.025	73.259	1.00	7.01
ATOM	1518	CB	ARG 1 188	41.205	-6.560	74.913	1.00	7.01

129/208

ATOM	1519	CG	ARG	1	188	41.182	-6.124	76.366	1.00	7.01
ATOM	1520	CD	ARG	1	188	39.731	-6.059	76.851	1.00	7.01
ATOM	1521	NE	ARG	1	188	38.929	-7.004	76.016	1.00	7.01
ATOM	1522	CZ	ARG	1	188	38.255	-6.572	74.908	1.00	7.01
ATOM	1523	NH1	ARG	1	188	37.581	-7.464	74.124	1.00	7.01
ATOM	1524	NH2	ARG	1	188	38.254	-5.248	74.577	1.00	7.01
ATOM	1525	N	PHE	1	189	43.383	-4.052	74.760	1.00	0.98
ATOM	1526	CA	PHE	1	189	43.478	-2.623	74.707	1.00	0.98
ATOM	1527	C	PHE	1	189	43.840	-2.264	73.303	1.00	0.98
ATOM	1528	O	PHE	1	189	43.277	-1.338	72.727	1.00	0.98
ATOM	1529	CB	PHE	1	189	44.545	-2.041	75.652	1.00	0.98
ATOM	1530	CG	PHE	1	189	44.534	-0.555	75.493	1.00	0.98
ATOM	1531	CD1	PHE	1	189	43.528	0.202	76.051	1.00	0.98
ATOM	1532	CD2	PHE	1	189	45.574	0.092	74.866	1.00	0.98
ATOM	1533	CE1	PHE	1	189	43.539	1.574	75.949	1.00	0.98
ATOM	1534	CE2	PHE	1	189	45.595	1.465	74.769	1.00	0.98
ATOM	1535	CZ	PHE	1	189	44.573	2.210	75.305	1.00	0.98
ATOM	1536	N	TYR	1	190	44.766	-3.023	72.695	1.00	0.91
ATOM	1537	CA	TYR	1	190	45.206	-2.741	71.360	1.00	0.91
ATOM	1538	C	TYR	1	190	44.049	-2.805	70.410	1.00	0.91
ATOM	1539	O	TYR	1	190	43.888	-1.932	69.560	1.00	0.91
ATOM	1540	CB	TYR	1	190	46.262	-3.757	70.893	1.00	0.91
ATOM	1541	CG	TYR	1	190	46.582	-3.521	69.457	1.00	0.91
ATOM	1542	CD1	TYR	1	190	47.439	-2.514	69.079	1.00	0.91
ATOM	1543	CD2	TYR	1	190	46.117	-4.395	68.501	1.00	0.91
ATOM	1544	CE1	TYR	1	190	47.814	-2.374	67.764	1.00	0.91
ATOM	1545	CE2	TYR	1	190	46.490	-4.261	67.185	1.00	0.91
ATOM	1546	CZ	TYR	1	190	47.350	-3.257	66.818	1.00	0.91
ATOM	1547	OH	TYR	1	190	47.742	-3.121	65.469	1.00	0.91
ATOM	1548	N	GLN	1	191	43.200	-3.839	70.545	1.00	1.02
ATOM	1549	CA	GLN	1	191	42.095	-4.033	69.649	1.00	1.02
ATOM	1550	C	GLN	1	191	41.114	-2.906	69.735	1.00	1.02
ATOM	1551	O	GLN	1	191	40.672	-2.376	68.716	1.00	1.02
ATOM	1552	CB	GLN	1	191	41.316	-5.320	69.969	1.00	1.02
ATOM	1553	CG	GLN	1	191	42.146	-6.595	69.816	1.00	1.02
ATOM	1554	CD	GLN	1	191	41.267	-7.774	70.212	1.00	1.02
ATOM	1555	OE1	GLN	1	191	40.666	-7.783	71.285	1.00	1.02
ATOM	1556	NE2	GLN	1	191	41.183	-8.796	69.319	1.00	1.02
ATOM	1557	N	LEU	1	192	40.749	-2.506	70.966	1.00	1.00
ATOM	1558	CA	LEU	1	192	39.760	-1.485	71.157	1.00	1.00
ATOM	1559	C	LEU	1	192	40.237	-0.166	70.656	1.00	1.00
ATOM	1560	O	LEU	1	192	39.487	0.592	70.042	1.00	1.00
ATOM	1561	CB	LEU	1	192	39.385	-1.308	72.632	1.00	1.00
ATOM	1562	CG	LEU	1	192	38.748	-2.573	73.226	1.00	1.00
ATOM	1563	CD1	LEU	1	192	38.380	-2.363	74.698	1.00	1.00
ATOM	1564	CD2	LEU	1	192	37.567	-3.057	72.370	1.00	1.00
ATOM	1565	N	THR	1	193	41.512	0.142	70.927	1.00	4.43
ATOM	1566	CA	THR	1	193	42.060	1.403	70.562	1.00	4.43
ATOM	1567	C	THR	1	193	42.166	1.477	69.075	1.00	4.43

130/208

ATOM	1568	O	THR	1	193	41.979	2.540	68.488	1.00	4.43
ATOM	1569	CB	THR	1	193	43.414	1.596	71.131	1.00	4.43
ATOM	1570	OG1	THR	1	193	43.458	1.208	72.490	1.00	4.43
ATOM	1571	CG2	THR	1	193	43.568	3.091	71.151	1.00	4.43
ATOM	1572	N	LYS	1	194	42.494	0.339	68.433	1.00	6.16
ATOM	1573	CA	LYS	1	194	42.623	0.290	67.005	1.00	6.16
ATOM	1574	C	LYS	1	194	41.296	0.583	66.383	1.00	6.16
ATOM	1575	O	LYS	1	194	41.212	1.253	65.356	1.00	6.16
ATOM	1576	CB	LYS	1	194	43.111	-1.073	66.484	1.00	6.16
ATOM	1577	CG	LYS	1	194	43.248	-1.117	64.961	1.00	6.16
ATOM	1578	CD	LYS	1	194	44.290	-0.151	64.396	1.00	6.16
ATOM	1579	CE	LYS	1	194	45.715	-0.698	64.418	1.00	6.16
ATOM	1580	NZ	LYS	1	194	46.183	-0.792	65.815	1.00	6.16
ATOM	1581	N	LEU	1	195	40.215	0.085	67.006	1.00	5.39
ATOM	1582	CA	LEU	1	195	38.888	0.303	66.507	1.00	5.39
ATOM	1583	C	LEU	1	195	38.613	1.771	66.485	1.00	5.39
ATOM	1584	O	LEU	1	195	38.054	2.295	65.522	1.00	5.39
ATOM	1585	CB	LEU	1	195	37.836	-0.398	67.397	1.00	5.39
ATOM	1586	CG	LEU	1	195	36.356	-0.035	67.146	1.00	5.39
ATOM	1587	CD1	LEU	1	195	35.993	1.320	67.763	1.00	5.39
ATOM	1588	CD2	LEU	1	195	35.993	-0.081	65.660	1.00	5.39
ATOM	1589	N	LEU	1	196	39.026	2.480	67.547	1.00	3.85
ATOM	1590	CA	LEU	1	196	38.718	3.870	67.649	1.00	3.85
ATOM	1591	C	LEU	1	196	39.453	4.591	66.553	1.00	3.85
ATOM	1592	O	LEU	1	196	38.899	5.472	65.896	1.00	3.85
ATOM	1593	CB	LEU	1	196	39.124	4.424	69.026	1.00	3.85
ATOM	1594	CG	LEU	1	196	38.270	5.615	69.496	1.00	3.85
ATOM	1595	CD1	LEU	1	196	38.931	6.355	70.668	1.00	3.85
ATOM	1596	CD2	LEU	1	196	37.816	6.507	68.337	1.00	3.85
ATOM	1597	N	ASP	1	197	40.727	4.227	66.300	1.00	5.56
ATOM	1598	CA	ASP	1	197	41.420	4.912	65.248	1.00	5.56
ATOM	1599	C	ASP	1	197	40.841	4.627	63.891	1.00	5.56
ATOM	1600	O	ASP	1	197	40.842	5.491	63.016	1.00	5.56
ATOM	1601	CB	ASP	1	197	42.966	4.858	65.312	1.00	5.56
ATOM	1602	CG	ASP	1	197	43.553	3.465	65.392	1.00	5.56
ATOM	1603	OD1	ASP	1	197	44.144	3.024	64.378	1.00	5.56
ATOM	1604	OD2	ASP	1	197	43.477	2.844	66.481	1.00	5.56
ATOM	1605	N	SER	1	198	40.292	3.417	63.689	1.00	0.90
ATOM	1606	CA	SER	1	198	39.691	3.047	62.437	1.00	0.90
ATOM	1607	C	SER	1	198	38.489	3.904	62.168	1.00	0.90
ATOM	1608	O	SER	1	198	38.138	4.154	61.015	1.00	0.90
ATOM	1609	CB	SER	1	198	39.224	1.580	62.412	1.00	0.90
ATOM	1610	OG	SER	1	198	40.339	0.709	62.538	1.00	0.90
ATOM	1611	N	MET	1	199	37.815	4.380	63.231	1.00	6.77
ATOM	1612	CA	MET	1	199	36.599	5.121	63.049	1.00	6.77
ATOM	1613	C	MET	1	199	36.816	6.395	62.286	1.00	6.77
ATOM	1614	O	MET	1	199	35.907	6.887	61.620	1.00	6.77
ATOM	1615	CB	MET	1	199	35.834	5.396	64.355	1.00	6.77
ATOM	1616	CG	MET	1	199	34.394	5.851	64.099	1.00	6.77

131/208

ATOM	1617	SD	MET	1	199	33.245	5.583	65.483	1.00	6.77
ATOM	1618	CE	MET	1	199	32.998	3.818	65.128	1.00	6.77
ATOM	1619	N	HIS	1	200	38.025	6.981	62.351	1.00	0.84
ATOM	1620	CA	HIS	1	200	38.228	8.211	61.639	1.00	0.84
ATOM	1621	C	HIS	1	200	37.937	8.046	60.180	1.00	0.84
ATOM	1622	O	HIS	1	200	37.260	8.881	59.582	1.00	0.84
ATOM	1623	CB	HIS	1	200	39.665	8.736	61.742	1.00	0.84
ATOM	1624	CG	HIS	1	200	40.009	9.172	63.128	1.00	0.84
ATOM	1625	ND1	HIS	1	200	40.741	8.424	64.024	1.00	0.84
ATOM	1626	CD2	HIS	1	200	39.683	10.322	63.777	1.00	0.84
ATOM	1627	CE1	HIS	1	200	40.831	9.159	65.160	1.00	0.84
ATOM	1628	NE2	HIS	1	200	40.208	10.319	65.056	1.00	0.84
ATOM	1629	N	GLU	1	201	38.438	6.964	59.560	1.00	5.71
ATOM	1630	CA	GLU	1	201	38.209	6.768	58.158	1.00	5.71
ATOM	1631	C	GLU	1	201	36.749	6.560	57.910	1.00	5.71
ATOM	1632	O	GLU	1	201	36.190	7.104	56.959	1.00	5.71
ATOM	1633	CB	GLU	1	201	38.951	5.541	57.601	1.00	5.71
ATOM	1634	CG	GLU	1	201	38.746	5.331	56.099	1.00	5.71
ATOM	1635	CD	GLU	1	201	39.521	6.414	55.364	1.00	5.71
ATOM	1636	OE1	GLU	1	201	39.482	6.417	54.105	1.00	5.71
ATOM	1637	OE2	GLU	1	201	40.162	7.254	56.051	1.00	5.71
ATOM	1638	N	VAL	1	202	36.085	5.767	58.774	1.00	4.12
ATOM	1639	CA	VAL	1	202	34.702	5.475	58.539	1.00	4.12
ATOM	1640	C	VAL	1	202	33.860	6.711	58.636	1.00	4.12
ATOM	1641	O	VAL	1	202	32.983	6.939	57.805	1.00	4.12
ATOM	1642	CB	VAL	1	202	34.121	4.440	59.465	1.00	4.12
ATOM	1643	CG1	VAL	1	202	34.911	3.132	59.287	1.00	4.12
ATOM	1644	CG2	VAL	1	202	34.084	4.979	60.901	1.00	4.12
ATOM	1645	N	VAL	1	203	34.128	7.562	59.642	1.00	3.85
ATOM	1646	CA	VAL	1	203	33.336	8.742	59.853	1.00	3.85
ATOM	1647	C	VAL	1	203	33.475	9.690	58.699	1.00	3.85
ATOM	1648	O	VAL	1	203	32.552	10.441	58.384	1.00	3.85
ATOM	1649	CB	VAL	1	203	33.684	9.470	61.121	1.00	3.85
ATOM	1650	CG1	VAL	1	203	35.042	10.170	60.960	1.00	3.85
ATOM	1651	CG2	VAL	1	203	32.527	10.419	61.461	1.00	3.85
ATOM	1652	N	GLU	1	204	34.643	9.682	58.032	1.00	3.18
ATOM	1653	CA	GLU	1	204	34.877	10.585	56.942	1.00	3.18
ATOM	1654	C	GLU	1	204	33.848	10.364	55.878	1.00	3.18
ATOM	1655	O	GLU	1	204	33.364	11.319	55.272	1.00	3.18
ATOM	1656	CB	GLU	1	204	36.260	10.392	56.298	1.00	3.18
ATOM	1657	CG	GLU	1	204	36.552	11.380	55.167	1.00	3.18
ATOM	1658	CD	GLU	1	204	37.941	11.076	54.626	1.00	3.18
ATOM	1659	OE1	GLU	1	204	38.216	9.881	54.339	1.00	3.18
ATOM	1660	OE2	GLU	1	204	38.749	12.036	54.497	1.00	3.18
ATOM	1661	N	ASN	1	205	33.491	9.094	55.610	1.00	0.60
ATOM	1662	CA	ASN	1	205	32.509	8.814	54.601	1.00	0.60
ATOM	1663	C	ASN	1	205	31.180	9.372	55.011	1.00	0.60
ATOM	1664	O	ASN	1	205	30.443	9.899	54.180	1.00	0.60
ATOM	1665	CB	ASN	1	205	32.342	7.311	54.324	1.00	0.60

132/208

ATOM 1666 CG ASN 1 205	33.573	6.857	53.551	1.00	0.60
ATOM 1667 OD1 ASN 1 205	33.971	7.491	52.575	1.00	0.60
ATOM 1668 ND2 ASN 1 205	34.200	5.737	54.000	1.00	0.60
ATOM 1669 N LEU 1 206	30.833	9.263	56.308	1.00	3.88
ATOM 1670 CA LEU 1 206	29.590	9.801	56.792	1.00	3.88
ATOM 1671 C LEU 1 206	29.590	11.288	56.603	1.00	3.88
ATOM 1672 O LEU 1 206	28.594	11.876	56.185	1.00	3.88
ATOM 1673 CB LEU 1 206	29.374	9.562	58.302	1.00	3.88
ATOM 1674 CG LEU 1 206	28.910	8.147	58.708	1.00	3.88
ATOM 1675 CD1 LEU 1 206	27.419	7.956	58.399	1.00	3.88
ATOM 1676 CD2 LEU 1 206	29.780	7.041	58.090	1.00	3.88
ATOM 1677 N LEU 1 207	30.728	11.935	56.906	1.00	4.19
ATOM 1678 CA LEU 1 207	30.855	13.361	56.816	1.00	4.19
ATOM 1679 C LEU 1 207	30.630	13.821	55.409	1.00	4.19
ATOM 1680 O LEU 1 207	29.925	14.802	55.175	1.00	4.19
ATOM 1681 CB LEU 1 207	32.253	13.792	57.322	1.00	4.19
ATOM 1682 CG LEU 1 207	32.675	15.259	57.113	1.00	4.19
ATOM 1683 CD1 LEU 1 207	33.895	15.597	57.985	1.00	4.19
ATOM 1684 CD2 LEU 1 207	33.001	15.538	55.636	1.00	4.19
ATOM 1685 N ASN 1 208	31.222	13.114	54.431	1.00	1.53
ATOM 1686 CA ASN 1 208	31.089	13.501	53.056	1.00	1.53
ATOM 1687 C ASN 1 208	29.664	13.377	52.611	1.00	1.53
ATOM 1688 O ASN 1 208	29.136	14.262	51.940	1.00	1.53
ATOM 1689 CB ASN 1 208	31.935	12.625	52.115	1.00	1.53
ATOM 1690 CG ASN 1 208	33.402	12.887	52.423	1.00	1.53
ATOM 1691 OD1 ASN 1 208	34.144	11.976	52.787	1.00	1.53
ATOM 1692 ND2 ASN 1 208	33.835	14.168	52.275	1.00	1.53
ATOM 1693 N TYR 1 209	28.999	12.269	52.989	1.00	0.82
ATOM 1694 CA TYR 1 209	27.651	12.014	52.564	1.00	0.82
ATOM 1695 C TYR 1 209	26.759	13.093	53.100	1.00	0.82
ATOM 1696 O TYR 1 209	25.914	13.623	52.379	1.00	0.82
ATOM 1697 CB TYR 1 209	27.142	10.657	53.088	1.00	0.82
ATOM 1698 CG TYR 1 209	25.798	10.364	52.512	1.00	0.82
ATOM 1699 CD1 TYR 1 209	24.653	10.876	53.079	1.00	0.82
ATOM 1700 CD2 TYR 1 209	25.682	9.497	51.449	1.00	0.82
ATOM 1701 CE1 TYR 1 209	23.415	10.537	52.584	1.00	0.82
ATOM 1702 CE2 TYR 1 209	24.447	9.155	50.950	1.00	0.82
ATOM 1703 CZ TYR 1 209	23.310	9.673	51.520	1.00	0.82
ATOM 1704 OH TYR 1 209	22.042	9.316	51.016	1.00	0.82
ATOM 1705 N CYS 1 210	26.937	13.457	54.387	1.00	3.72
ATOM 1706 CA CYS 1 210	26.103	14.462	54.986	1.00	3.72
ATOM 1707 C CYS 1 210	26.255	15.798	54.337	1.00	3.72
ATOM 1708 O CYS 1 210	25.267	16.467	54.042	1.00	3.72
ATOM 1709 CB CYS 1 210	26.370	14.703	56.480	1.00	3.72
ATOM 1710 SG CYS 1 210	25.473	13.553	57.554	1.00	3.72
ATOM 1711 N PHE 1 211	27.504	16.221	54.089	1.00	3.96
ATOM 1712 CA PHE 1 211	27.729	17.524	53.538	1.00	3.96
ATOM 1713 C PHE 1 211	27.103	17.603	52.183	1.00	3.96
ATOM 1714 O PHE 1 211	26.519	18.623	51.821	1.00	3.96

133/208

ATOM 1715 CB PHE 1 211	29.226	17.848	53.386	1.00	3.96
ATOM 1716 CG PHE 1 211	29.342	19.260	52.924	1.00	3.96
ATOM 1717 CD1 PHE 1 211	29.233	19.575	51.590	1.00	3.96
ATOM 1718 CD2 PHE 1 211	29.575	20.268	53.831	1.00	3.96
ATOM 1719 CE1 PHE 1 211	29.352	20.879	51.167	1.00	3.96
ATOM 1720 CE2 PHE 1 211	29.695	21.573	53.415	1.00	3.96
ATOM 1721 CZ PHE 1 211	29.584	21.880	52.080	1.00	3.96
ATOM 1722 N GLN 1 212	27.218	16.519	51.393	1.00	0.53
ATOM 1723 CA GLN 1 212	26.678	16.508	50.064	1.00	0.53
ATOM 1724 C GLN 1 212	25.187	16.643	50.107	1.00	0.53
ATOM 1725 O GLN 1 212	24.606	17.437	49.370	1.00	0.53
ATOM 1726 CB GLN 1 212	26.989	15.200	49.317	1.00	0.53
ATOM 1727 CG GLN 1 212	28.483	14.969	49.083	1.00	0.53
ATOM 1728 CD GLN 1 212	28.642	13.649	48.342	1.00	0.53
ATOM 1729 OE1 GLN 1 212	27.660	12.976	48.030	1.00	0.53
ATOM 1730 NE2 GLN 1 212	29.913	13.265	48.052	1.00	0.53
ATOM 1731 N THR 1 213	24.529	15.873	50.993	1.00	0.65
ATOM 1732 CA THR 1 213	23.097	15.882	51.086	1.00	0.65
ATOM 1733 C THR 1 213	22.633	17.223	51.556	1.00	0.65
ATOM 1734 O THR 1 213	21.580	17.711	51.145	1.00	0.65
ATOM 1735 CB THR 1 213	22.573	14.864	52.051	1.00	0.65
ATOM 1736 OG1 THR 1 213	22.993	13.564	51.664	1.00	0.65
ATOM 1737 CG2 THR 1 213	21.039	14.939	52.041	1.00	0.65
ATOM 1738 N PHE 1 214	23.418	17.846	52.452	1.00	0.68
ATOM 1739 CA PHE 1 214	23.086	19.118	53.022	1.00	0.68
ATOM 1740 C PHE 1 214	22.996	20.140	51.926	1.00	0.68
ATOM 1741 O PHE 1 214	22.048	20.921	51.873	1.00	0.68
ATOM 1742 CB PHE 1 214	24.168	19.561	54.028	1.00	0.68
ATOM 1743 CG PHE 1 214	23.759	20.819	54.713	1.00	0.68
ATOM 1744 CD1 PHE 1 214	22.913	20.778	55.798	1.00	0.68
ATOM 1745 CD2 PHE 1 214	24.320	22.023	54.351	1.00	0.68
ATOM 1746 CE1 PHE 1 214	22.605	21.926	56.490	1.00	0.68
ATOM 1747 CE2 PHE 1 214	24.016	23.173	55.039	1.00	0.68
ATOM 1748 CZ PHE 1 214	23.156	23.126	56.110	1.00	0.68
ATOM 1749 N LEU 1 215	23.986	20.159	51.013	1.00	6.34
ATOM 1750 CA LEU 1 215	23.981	21.102	49.927	1.00	6.34
ATOM 1751 C LEU 1 215	22.856	20.758	48.986	1.00	6.34
ATOM 1752 O LEU 1 215	22.184	21.629	48.435	1.00	6.34
ATOM 1753 CB LEU 1 215	25.301	21.078	49.135	1.00	6.34
ATOM 1754 CG LEU 1 215	25.355	22.077	47.965	1.00	6.34
ATOM 1755 CD1 LEU 1 215	25.292	23.529	48.468	1.00	6.34
ATOM 1756 CD2 LEU 1 215	26.579	21.817	47.073	1.00	6.34
ATOM 1757 N ASP 1 216	22.653	19.440	48.808	1.00	3.90
ATOM 1758 CA ASP 1 216	21.725	18.719	47.975	1.00	3.90
ATOM 1759 C ASP 1 216	20.330	18.794	48.524	1.00	3.90
ATOM 1760 O ASP 1 216	19.397	18.265	47.924	1.00	3.90
ATOM 1761 CB ASP 1 216	22.104	17.232	47.855	1.00	3.90
ATOM 1762 CG ASP 1 216	21.375	16.629	46.662	1.00	3.90
ATOM 1763 OD1 ASP 1 216	20.696	17.393	45.926	1.00	3.90

134/208

ATOM	1764	OD2 ASP 1 216	21.495	15.389	46.468	1.00	3.90
ATOM	1765	N LYS 1 217	20.165	19.463	49.680	1.00	3.84
ATOM	1766	CA LYS 1 217	18.980	19.529	50.495	1.00	3.84
ATOM	1767	C LYS 1 217	17.745	19.722	49.660	1.00	3.84
ATOM	1768	O LYS 1 217	16.658	19.309	50.062	1.00	3.84
ATOM	1769	CB LYS 1 217	19.089	20.703	51.485	1.00	3.84
ATOM	1770	CG LYS 1 217	17.973	20.790	52.519	1.00	3.84
ATOM	1771	CD LYS 1 217	18.318	21.703	53.696	1.00	3.84
ATOM	1772	CE LYS 1 217	17.234	21.758	54.772	1.00	3.84
ATOM	1773	NZ LYS 1 217	17.690	22.596	55.904	1.00	3.84
ATOM	1774	N THR 1 218	17.873	20.315	48.459	1.00	5.26
ATOM	1775	CA THR 1 218	16.766	20.514	47.558	1.00	5.26
ATOM	1776	C THR 1 218	16.108	19.182	47.278	1.00	5.26
ATOM	1777	O THR 1 218	14.979	19.132	46.791	1.00	5.26
ATOM	1778	CB THR 1 218	17.160	21.119	46.242	1.00	5.26
ATOM	1779	OG1 THR 1 218	16.001	21.528	45.529	1.00	5.26
ATOM	1780	CG2 THR 1 218	17.941	20.077	45.425	1.00	5.26
ATOM	1781	N MET 1 219	16.808	18.067	47.597	1.00	6.69
ATOM	1782	CA MET 1 219	16.430	16.677	47.470	1.00	6.69
ATOM	1783	C MET 1 219	15.188	16.447	48.280	1.00	6.69
ATOM	1784	O MET 1 219	14.613	15.356	48.276	1.00	6.69
ATOM	1785	CB MET 1 219	17.524	15.707	47.938	1.00	6.69
ATOM	1786	CG MET 1 219	17.292	14.281	47.443	1.00	6.69
ATOM	1787	SD MET 1 219	17.338	14.138	45.631	1.00	6.69
ATOM	1788	CE MET 1 219	19.001	14.846	45.455	1.00	6.69
ATOM	1789	N SER 1 220	14.809	17.467	49.072	1.00	4.00
ATOM	1790	CA SER 1 220	13.621	17.455	49.863	1.00	4.00
ATOM	1791	C SER 1 220	13.977	16.815	51.147	1.00	4.00
ATOM	1792	O SER 1 220	13.140	16.226	51.829	1.00	4.00
ATOM	1793	CB SER 1 220	12.434	16.720	49.215	1.00	4.00
ATOM	1794	OG SER 1 220	11.988	17.433	48.070	1.00	4.00
ATOM	1795	N ILE 1 221	15.270	16.937	51.492	1.00	4.77
ATOM	1796	CA ILE 1 221	15.760	16.481	52.750	1.00	4.77
ATOM	1797	C ILE 1 221	15.799	17.683	53.634	1.00	4.77
ATOM	1798	O ILE 1 221	16.357	18.715	53.274	1.00	4.77
ATOM	1799	CB ILE 1 221	17.158	15.938	52.702	1.00	4.77
ATOM	1800	CG1 ILE 1 221	17.582	15.490	54.109	1.00	4.77
ATOM	1801	CG2 ILE 1 221	18.086	16.978	52.051	1.00	4.77
ATOM	1802	CD1 ILE 1 221	18.995	14.921	54.165	1.00	4.77
ATOM	1803	N GLU 1 222	15.194	17.590	54.828	1.00	2.49
ATOM	1804	CA GLU 1 222	15.181	18.727	55.697	1.00	2.49
ATOM	1805	C GLU 1 222	16.154	18.509	56.812	1.00	2.49
ATOM	1806	O GLU 1 222	16.209	17.431	57.400	1.00	2.49
ATOM	1807	CB GLU 1 222	13.785	18.987	56.299	1.00	2.49
ATOM	1808	CG GLU 1 222	13.710	20.127	57.317	1.00	2.49
ATOM	1809	CD GLU 1 222	13.663	19.508	58.708	1.00	2.49
ATOM	1810	OE1 GLU 1 222	14.638	18.802	59.081	1.00	2.49
ATOM	1811	OE2 GLU 1 222	12.643	19.728	59.417	1.00	2.49
ATOM	1812	N PHE 1 223	16.977	19.540	57.101	1.00	0.93



135/208

ATOM 1813	CA PHE 1 223	17.919	19.483	58.185	1.00	0.93
ATOM 1814	C PHE 1 223	17.459	20.474	59.211	1.00	0.93
ATOM 1815	O PHE 1 223	17.096	21.603	58.886	1.00	0.93
ATOM 1816	CB PHE 1 223	19.359	19.891	57.805	1.00	0.93
ATOM 1817	CG PHE 1 223	20.012	18.809	57.010	1.00	0.93
ATOM 1818	CD1 PHE 1 223	19.727	18.645	55.674	1.00	0.93
ATOM 1819	CD2 PHE 1 223	21.011	18.046	57.574	1.00	0.93
ATOM 1820	CE1 PHE 1 223	20.394	17.701	54.928	1.00	0.93
ATOM 1821	CE2 PHE 1 223	21.686	17.104	56.833	1.00	0.93
ATOM 1822	CZ PHE 1 223	21.372	16.927	55.507	1.00	0.93
ATOM 1823	N PRO 1 224	17.471	20.069	60.453	1.00	5.86
ATOM 1824	CA PRO 1 224	17.050	20.922	61.534	1.00	5.86
ATOM 1825	C PRO 1 224	18.090	21.970	61.789	1.00	5.86
ATOM 1826	O PRO 1 224	19.202	21.841	61.282	1.00	5.86
ATOM 1827	CB PRO 1 224	16.789	19.996	62.727	1.00	5.86
ATOM 1828	CG PRO 1 224	17.402	18.643	62.320	1.00	5.86
ATOM 1829	CD PRO 1 224	17.344	18.662	60.787	1.00	5.86
ATOM 1830	N GLU 1 225	17.739	23.020	62.559	1.00	2.88
ATOM 1831	CA GLU 1 225	18.615	24.135	62.793	1.00	2.88
ATOM 1832	C GLU 1 225	19.892	23.801	63.507	1.00	2.88
ATOM 1833	O GLU 1 225	20.962	24.232	63.082	1.00	2.88
ATOM 1834	CB GLU 1 225	17.942	25.263	63.597	1.00	2.88
ATOM 1835	CG GLU 1 225	16.853	26.013	62.825	1.00	2.88
ATOM 1836	CD GLU 1 225	15.579	25.180	62.839	1.00	2.88
ATOM 1837	OE1 GLU 1 225	15.375	24.422	63.825	1.00	2.88
ATOM 1838	OE2 GLU 1 225	14.790	25.294	61.863	1.00	2.88
ATOM 1839	N MET 1 226	19.833	23.028	64.608	1.00	6.09
ATOM 1840	CA MET 1 226	21.035	22.758	65.350	1.00	6.09
ATOM 1841	C MET 1 226	22.000	21.956	64.535	1.00	6.09
ATOM 1842	O MET 1 226	23.203	22.213	64.549	1.00	6.09
ATOM 1843	CB MET 1 226	20.783	21.997	66.666	1.00	6.09
ATOM 1844	CG MET 1 226	20.163	20.610	66.483	1.00	6.09
ATOM 1845	SD MET 1 226	18.403	20.624	66.032	1.00	6.09
ATOM 1846	CE MET 1 226	17.830	20.977	67.719	1.00	6.09
ATOM 1847	N LEU 1 227	21.491	20.948	63.806	1.00	0.72
ATOM 1848	CA LEU 1 227	22.336	20.113	63.004	1.00	0.72
ATOM 1849	C LEU 1 227	22.918	20.921	61.894	1.00	0.72
ATOM 1850	O LEU 1 227	24.082	20.756	61.533	1.00	0.72
ATOM 1851	CB LEU 1 227	21.582	18.934	62.364	1.00	0.72
ATOM 1852	CG LEU 1 227	22.481	18.028	61.504	1.00	0.72
ATOM 1853	CD1 LEU 1 227	23.563	17.344	62.352	1.00	0.72
ATOM 1854	CD2 LEU 1 227	21.647	17.030	60.684	1.00	0.72
ATOM 1855	N ALA 1 228	22.109	21.828	61.320	1.00	0.66
ATOM 1856	CA ALA 1 228	22.574	22.629	60.228	1.00	0.66
ATOM 1857	C ALA 1 228	23.726	23.463	60.695	1.00	0.66
ATOM 1858	O ALA 1 228	24.706	23.638	59.972	1.00	0.66
ATOM 1859	CB ALA 1 228	21.497	23.587	59.693	1.00	0.66
ATOM 1860	N GLU 1 229	23.645	24.002	61.925	1.00	4.93
ATOM 1861	CA GLU 1 229	24.691	24.869	62.386	1.00	4.93

136/208

ATOM	1862	C	GLU 1 229	25.999	24.149	62.529	1.00	4.93
ATOM	1863	O	GLU 1 229	27.039	24.667	62.125	1.00	4.93
ATOM	1864	CB	GLU 1 229	24.358	25.573	63.719	1.00	4.93
ATOM	1865	CG	GLU 1 229	24.354	24.672	64.954	1.00	4.93
ATOM	1866	CD	GLU 1 229	25.721	24.784	65.612	1.00	4.93
ATOM	1867	OE1	GLU 1 229	26.063	23.879	66.419	1.00	4.93
ATOM	1868	OE2	GLU 1 229	26.440	25.778	65.321	1.00	4.93
ATOM	1869	N	ILE 1 230	25.992	22.927	63.095	1.00	5.97
ATOM	1870	CA	ILE 1 230	27.224	22.216	63.298	1.00	5.97
ATOM	1871	C	ILE 1 230	27.828	21.845	61.978	1.00	5.97
ATOM	1872	O	ILE 1 230	29.046	21.898	61.806	1.00	5.97
ATOM	1873	CB	ILE 1 230	27.042	20.975	64.125	1.00	5.97
ATOM	1874	CG1	ILE 1 230	28.399	20.479	64.647	1.00	5.97
ATOM	1875	CG2	ILE 1 230	26.271	19.943	63.286	1.00	5.97
ATOM	1876	CD1	ILE 1 230	28.275	19.512	65.823	1.00	5.97
ATOM	1877	N	ILE 1 231	26.982	21.458	61.005	1.00	3.96
ATOM	1878	CA	ILE 1 231	27.466	21.066	59.710	1.00	3.96
ATOM	1879	C	ILE 1 231	28.172	22.240	59.102	1.00	3.96
ATOM	1880	O	ILE 1 231	29.322	22.149	58.675	1.00	3.96
ATOM	1881	CB	ILE 1 231	26.339	20.766	58.749	1.00	3.96
ATOM	1882	CG1	ILE 1 231	25.418	19.622	59.220	1.00	3.96
ATOM	1883	CG2	ILE 1 231	26.972	20.489	57.375	1.00	3.96
ATOM	1884	CD1	ILE 1 231	26.017	18.227	59.087	1.00	3.96
ATOM	1885	N	THR 1 232	27.496	23.400	59.089	1.00	0.77
ATOM	1886	CA	THR 1 232	28.027	24.564	58.444	1.00	0.77
ATOM	1887	C	THR 1 232	29.275	25.027	59.109	1.00	0.77
ATOM	1888	O	THR 1 232	30.232	25.418	58.442	1.00	0.77
ATOM	1889	CB	THR 1 232	27.062	25.713	58.456	1.00	0.77
ATOM	1890	OG1	THR 1 232	25.861	25.351	57.791	1.00	0.77
ATOM	1891	CG2	THR 1 232	27.716	26.913	57.749	1.00	0.77
ATOM	1892	N	ASN 1 233	29.303	25.013	60.451	1.00	2.07
ATOM	1893	CA	ASN 1 233	30.466	25.538	61.089	1.00	2.07
ATOM	1894	C	ASN 1 233	31.704	24.742	60.810	1.00	2.07
ATOM	1895	O	ASN 1 233	32.734	25.302	60.450	1.00	2.07
ATOM	1896	CB	ASN 1 233	30.309	25.644	62.614	1.00	2.07
ATOM	1897	CG	ASN 1 233	29.322	26.763	62.916	1.00	2.07
ATOM	1898	OD1	ASN 1 233	28.277	26.880	62.278	1.00	2.07
ATOM	1899	ND2	ASN 1 233	29.668	27.620	63.914	1.00	2.07
ATOM	1900	N	GLN 1 234	31.676	23.431	61.097	1.00	2.81
ATOM	1901	CA	GLN 1 234	32.824	22.592	60.914	1.00	2.81
ATOM	1902	C	GLN 1 234	33.052	21.633	59.765	1.00	2.81
ATOM	1903	O	GLN 1 234	34.201	21.356	59.425	1.00	2.81
ATOM	1904	CB	GLN 1 234	33.166	21.915	62.226	1.00	2.81
ATOM	1905	CG	GLN 1 234	33.523	22.907	63.332	1.00	2.81
ATOM	1906	CD	GLN 1 234	34.798	23.627	62.926	1.00	2.81
ATOM	1907	OE1	GLN 1 234	35.186	24.630	63.522	1.00	2.81
ATOM	1908	NE2	GLN 1 234	35.473	23.099	61.873	1.00	2.81
ATOM	1909	N	ILE 1 235	31.996	21.074	59.135	1.00	7.20
ATOM	1910	CA	ILE 1 235	32.227	19.974	58.228	1.00	7.20

SUBSTITUTE SHEET (RULE 26)

137/208

ATOM 1911 C ILE 1 235	33.138	20.265	57.073	1.00	7.20
ATOM 1912 O ILE 1 235	33.936	19.389	56.735	1.00	7.20
ATOM 1913 CB ILE 1 235	30.964	19.231	57.793	1.00	7.20
ATOM 1914 CG1 ILE 1 235	31.296	17.943	57.019	1.00	7.20
ATOM 1915 CG2 ILE 1 235	30.038	20.138	56.975	1.00	7.20
ATOM 1916 CD1 ILE 1 235	31.720	18.184	55.569	1.00	7.20
ATOM 1917 N PRO 1 236	33.124	21.394	56.428	1.00	1.16
ATOM 1918 CA PRO 1 236	34.020	21.577	55.326	1.00	1.16
ATOM 1919 C PRO 1 236	35.435	21.530	55.806	1.00	1.16
ATOM 1920 O PRO 1 236	36.296	21.042	55.076	1.00	1.16
ATOM 1921 CB PRO 1 236	33.632	22.909	54.688	1.00	1.16
ATOM 1922 CG PRO 1 236	32.150	23.083	55.073	1.00	1.16
ATOM 1923 CD PRO 1 236	32.015	22.333	56.408	1.00	1.16
ATOM 1924 N LYS 1 237	35.698	22.041	57.025	1.00	4.23
ATOM 1925 CA LYS 1 237	37.028	22.057	57.557	1.00	4.23
ATOM 1926 C LYS 1 237	37.491	20.659	57.812	1.00	4.23
ATOM 1927 O LYS 1 237	38.618	20.303	57.473	1.00	4.23
ATOM 1928 CB LYS 1 237	37.154	22.792	58.903	1.00	4.23
ATOM 1929 CG LYS 1 237	36.913	24.300	58.836	1.00	4.23
ATOM 1930 CD LYS 1 237	36.890	24.960	60.217	1.00	4.23
ATOM 1931 CE LYS 1 237	36.604	26.462	60.190	1.00	4.23
ATOM 1932 NZ LYS 1 237	35.143	26.695	60.175	1.00	4.23
ATOM 1933 N TYR 1 238	36.620	19.820	58.410	1.00	1.32
ATOM 1934 CA TYR 1 238	37.004	18.473	58.743	1.00	1.32
ATOM 1935 C TYR 1 238	37.385	17.756	57.503	1.00	1.32
ATOM 1936 O TYR 1 238	38.418	17.094	57.438	1.00	1.32
ATOM 1937 CB TYR 1 238	35.862	17.534	59.149	1.00	1.32
ATOM 1938 CG TYR 1 238	35.233	18.013	60.377	1.00	1.32
ATOM 1939 CD1 TYR 1 238	35.842	17.772	61.578	1.00	1.32
ATOM 1940 CD2 TYR 1 238	34.006	18.620	60.309	1.00	1.32
ATOM 1941 CE1 TYR 1 238	35.279	18.269	62.716	1.00	1.32
ATOM 1942 CE2 TYR 1 238	33.436	19.101	61.451	1.00	1.32
ATOM 1943 CZ TYR 1 238	34.106	18.973	62.640	1.00	1.32
ATOM 1944 OH TYR 1 238	33.673	19.698	63.760	1.00	1.32
ATOM 1945 N SER 1 239	36.514	17.867	56.489	1.00	3.15
ATOM 1946 CA SER 1 239	36.681	17.123	55.279	1.00	3.15
ATOM 1947 C SER 1 239	37.975	17.507	54.646	1.00	3.15
ATOM 1948 O SER 1 239	38.677	16.668	54.084	1.00	3.15
ATOM 1949 CB SER 1 239	35.564	17.398	54.258	1.00	3.15
ATOM 1950 OG SER 1 239	35.780	16.633	53.081	1.00	3.15
ATOM 1951 N ASN 1 240	38.318	18.802	54.734	1.00	0.86
ATOM 1952 CA ASN 1 240	39.522	19.324	54.162	1.00	0.86
ATOM 1953 C ASN 1 240	40.702	18.696	54.842	1.00	0.86
ATOM 1954 O ASN 1 240	41.765	18.555	54.242	1.00	0.86
ATOM 1955 CB ASN 1 240	39.644	20.850	54.319	1.00	0.86
ATOM 1956 CG ASN 1 240	38.554	21.496	53.475	1.00	0.86
ATOM 1957 OD1 ASN 1 240	38.152	20.962	52.442	1.00	0.86
ATOM 1958 ND2 ASN 1 240	38.059	22.679	53.925	1.00	0.86
ATOM 1959 N GLY 1 241	40.561	18.294	56.119	1.00	0.83

138/208

ATOM	1960	CA	GLY 1 241	41.697	17.718	56.787	1.00	0.83
ATOM	1961	C	GLY 1 241	42.399	18.795	57.555	1.00	0.83
ATOM	1962	O	GLY 1 241	43.590	18.708	57.850	1.00	0.83
ATOM	1963	N	ASN 1 242	41.635	19.849	57.875	1.00	2.92
ATOM	1964	CA	ASN 1 242	42.002	21.027	58.606	1.00	2.92
ATOM	1965	C	ASN 1 242	42.169	20.756	60.070	1.00	2.92
ATOM	1966	O	ASN 1 242	42.453	21.686	60.813	1.00	2.92
ATOM	1967	CB	ASN 1 242	40.955	22.145	58.488	1.00	2.92
ATOM	1968	CG	ASN 1 242	40.942	22.624	57.046	1.00	2.92
ATOM	1969	OD1	ASN 1 242	40.035	23.340	56.624	1.00	2.92
ATOM	1970	ND2	ASN 1 242	41.975	22.212	56.264	1.00	2.92
ATOM	1971	N	ILE 1 243	41.868	19.533	60.551	1.00	9.49
ATOM	1972	CA	ILE 1 243	41.910	19.235	61.960	1.00	9.49
ATOM	1973	C	ILE 1 243	42.936	18.170	62.206	1.00	9.49
ATOM	1974	O	ILE 1 243	43.381	17.497	61.278	1.00	9.49
ATOM	1975	CB	ILE 1 243	40.570	18.707	62.420	1.00	9.49
ATOM	1976	CG1	ILE 1 243	39.491	19.762	62.159	1.00	9.49
ATOM	1977	CG2	ILE 1 243	40.625	18.309	63.901	1.00	9.49
ATOM	1978	CD1	ILE 1 243	39.734	21.041	62.954	1.00	9.49
ATOM	1979	N	LYS 1 244	43.387	18.011	63.470	1.00	6.69
ATOM	1980	CA	LYS 1 244	44.315	16.949	63.696	1.00	6.69
ATOM	1981	C	LYS 1 244	43.670	15.828	64.449	1.00	6.69
ATOM	1982	O	LYS 1 244	43.232	15.951	65.587	1.00	6.69
ATOM	1983	CB	LYS 1 244	45.660	17.380	64.330	1.00	6.69
ATOM	1984	CG	LYS 1 244	45.628	18.055	65.702	1.00	6.69
ATOM	1985	CD	LYS 1 244	45.487	17.102	66.888	1.00	6.69
ATOM	1986	CE	LYS 1 244	44.224	17.349	67.705	1.00	6.69
ATOM	1987	NZ	LYS 1 244	44.078	16.337	68.763	1.00	6.69
ATOM	1988	N	LYS 1 245	43.565	14.675	63.771	1.00	7.88
ATOM	1989	CA	LYS 1 245	42.994	13.498	64.343	1.00	7.88
ATOM	1990	C	LYS 1 245	43.983	12.850	65.261	1.00	7.88
ATOM	1991	O	LYS 1 245	45.162	12.739	64.936	1.00	7.88
ATOM	1992	CB	LYS 1 245	42.480	12.569	63.221	1.00	7.88
ATOM	1993	CG	LYS 1 245	42.550	11.058	63.427	1.00	7.88
ATOM	1994	CD	LYS 1 245	43.799	10.426	62.802	1.00	7.88
ATOM	1995	CE	LYS 1 245	45.020	10.292	63.705	1.00	7.88
ATOM	1996	NZ	LYS 1 245	46.153	9.761	62.911	1.00	7.88
ATOM	1997	N	LEU 1 246	43.525	12.433	66.461	1.00	1.24
ATOM	1998	CA	LEU 1 246	44.406	11.806	67.410	1.00	1.24
ATOM	1999	C	LEU 1 246	44.362	10.349	67.118	1.00	1.24
ATOM	2000	O	LEU 1 246	43.285	9.777	66.956	1.00	1.24
ATOM	2001	CB	LEU 1 246	43.975	11.978	68.876	1.00	1.24
ATOM	2002	CG	LEU 1 246	44.138	13.418	69.380	1.00	1.24
ATOM	2003	CD1	LEU 1 246	43.705	13.561	70.848	1.00	1.24
ATOM	2004	CD2	LEU 1 246	45.582	13.893	69.147	1.00	1.24
ATOM	2005	N	LEU 1 247	45.546	9.712	67.038	1.00	6.31
ATOM	2006	CA	LEU 1 247	45.532	8.332	66.672	1.00	6.31
ATOM	2007	C	LEU 1 247	46.366	7.621	67.690	1.00	6.31
ATOM	2008	O	LEU 1 247	47.468	8.058	68.016	1.00	6.31

139/208

ATOM	2009	CB	LEU	1	247	46.199	8.117	65.308	1.00	6.31
ATOM	2010	CG	LEU	1	247	45.682	6.894	64.552	1.00	6.31
ATOM	2011	CD1	LEU	1	247	45.821	5.604	65.373	1.00	6.31
ATOM	2012	CD2	LEU	1	247	44.263	7.166	64.025	1.00	6.31
ATOM	2013	N	PHE	1	248	45.836	6.519	68.249	1.00	1.30
ATOM	2014	CA	PHE	1	248	46.539	5.746	69.229	1.00	1.30
ATOM	2015	C	PHE	1	248	47.648	4.947	68.648	1.00	1.30
ATOM	2016	O	PHE	1	248	48.649	4.687	69.313	1.00	1.30
ATOM	2017	CB	PHE	1	248	45.620	4.819	69.985	1.00	1.30
ATOM	2018	CG	PHE	1	248	44.791	5.716	70.834	1.00	1.30
ATOM	2019	CD1	PHE	1	248	45.240	6.092	72.080	1.00	1.30
ATOM	2020	CD2	PHE	1	248	43.504	6.020	70.458	1.00	1.30
ATOM	2021	CE1	PHE	1	248	44.419	6.778	72.942	1.00	1.30
ATOM	2022	CE2	PHE	1	248	42.682	6.713	71.314	1.00	1.30
ATOM	2023	CZ	PHE	1	248	43.133	7.075	72.562	1.00	1.30
ATOM	2024	N	HIS	1	249	47.487	4.497	67.396	1.00	3.57
ATOM	2025	CA	HIS	1	249	48.517	3.689	66.830	1.00	3.57
ATOM	2026	C	HIS	1	249	49.182	4.514	65.786	1.00	3.57
ATOM	2027	O	HIS	1	249	48.535	5.300	65.096	1.00	3.57
ATOM	2028	CB	HIS	1	249	47.959	2.401	66.206	1.00	3.57
ATOM	2029	CG	HIS	1	249	47.126	1.638	67.200	1.00	3.57
ATOM	2030	ND1	HIS	1	249	45.750	1.671	67.235	1.00	3.57
ATOM	2031	CD2	HIS	1	249	47.501	0.877	68.264	1.00	3.57
ATOM	2032	CE1	HIS	1	249	45.364	0.929	68.304	1.00	3.57
ATOM	2033	NE2	HIS	1	249	46.393	0.428	68.961	1.00	3.57
ATOM	2034	N	GLN	1	250	50.513	4.352	65.668	1.00	3.06
ATOM	2035	CA	GLN	1	250	51.307	5.130	64.766	1.00	3.06
ATOM	2036	C	GLN	1	250	50.873	4.894	63.360	1.00	3.06
ATOM	2037	O	GLN	1	250	49.793	4.366	63.101	1.00	3.06
ATOM	2038	CB	GLN	1	250	52.808	4.803	64.849	1.00	3.06
ATOM	2039	CG	GLN	1	250	53.426	5.104	66.217	1.00	3.06
ATOM	2040	CD	GLN	1	250	54.901	4.737	66.158	1.00	3.06
ATOM	2041	OE1	GLN	1	250	54.148	5.443	65.498	1.00	3.06
ATOM	2042	NE2	GLN	1	250	54.829	3.928	67.254	1.00	3.06
ATOM	2043	N	LYS	1	251	51.730	5.314	62.409	1.00	8.59
ATOM	2044	CA	LYS	1	251	51.464	5.195	61.006	1.00	8.59
ATOM	2045	C	LYS	1	251	50.081	5.753	60.685	1.00	8.59
ATOM	2046	O	LYS	1	251	49.467	6.412	61.567	1.00	8.59
ATOM	2047	CB	LYS	1	251	51.578	3.750	60.471	1.00	8.59
ATOM	2048	CG	LYS	1	251	50.546	2.755	61.013	1.00	8.59
ATOM	2049	CD	LYS	1	251	49.124	2.976	60.490	1.00	8.59
ATOM	2050	CE	LYS	1	251	49.003	2.835	58.971	1.00	8.59
ATOM	2051	NZ	LYS	1	251	47.603	3.062	58.549	1.00	8.59
ATOM	2052	OXT	LYS	1	251	49.624	5.533	59.532	1.00	8.59

END

140/208

Fig 14

Sequence alignment of ER and GR used for the conformation of the C-terminal -helix (helix 12) in a PR-based GR-model for the study of binding of antagonists.

gr_er	522	PATLPQLTPT	LVSLLLEVIEP	EVLYAGYDSS	VPDSTWRIMT	TLNMLGGRQV
lerr	307	ALSLTADQ	MVSALLDAEP	PILYSEYDPT	RPFSEASMMG	LLTNLADREL
		.+.	.+.	.+.	.+.	.+.
gr_er	572	IAAVKWAKAI	PGFRNLHLDD	QMTLLQYSWM	FLMAFALGWR	SYROSSANLL
lerr	355	VHMINWAKRV	PGFVDLTLHD	QVHLLECAWL	EILMIGLVWR	SMEHPG--KL
		.+.	.+.	.+.	.+.	.+.
gr_er	622	CFAPELLINE	QRMTLP-CMY	DQCKHMLYVS	SELHRLQVSY	EEYLCMKTLL
lerr	403	LFAPNLLDR	NQSKCVEGMV	EIFDMLLATS	SRFRMMNLQG	EEFVCLKSII
		.+.	.+.	.+.	.+.	.+.
gr_er	671	LLSSVPKDGL	KSQELFDEIR	MTYIKELGKA	IVKREG--NS	S-QNWQRFYQ
lerr	453	LLNSGVY---	---EEKDHIH	RVLDKITDTL	IHLMAKAGLT	LQQQHQRLAQ
		.+.	.+.	.+.	.+.	.+.
gr_er	718	LTKLLDSMHE	VVENLLNYCF	QTFLDKTMSI	EFPEMLAEII	TNQ
lerr	507	LLLILSHIRH	MSNKGMEHLY	SM-----P	L-YDLLLEML	DAH
		.+.	.+.	.+.	.+.	.+.

\* = identical amino acid residue

. = conservative amino acid substitution

141/208  
FIG. 15.

HEADER PROTEIN 28-FEB-100  
COMPND GR\_ER\_RAL  
AUTHOR GENERATED BY SYBYL, A PRODUCT OF TRIPOS, INC.  
SEQRES 1 1 240 PRO ALA THR LEU PRO GLN LEU THR PRO THR LEU VAL SER  
SEQRES 2 1 240 LEU LEU GLU VAL ILE GLU PRO GLU VAL LEU TYR ALA GLY  
SEQRES 3 1 240 TYR ASP SER SER VAL PRO ASP SER THR TRP ARG ILE MET  
SEQRES 4 1 240 THR THR LEU ASN MET LEU GLY GLY ARG GLN VAL ILE ALA  
SEQRES 5 1 240 ALA VAL LYS TRP ALA LYS ALA ILE PRO GLY PHE ARG ASN  
SEQRES 6 1 240 LEU HIS LEU ASP ASP GLN MET THR LEU LEU GLN TYR SER  
SEQRES 7 1 240 TRP MET PHE LEU MET ALA PHE ALA LEU GLY TRP ARG SER  
SEQRES 8 1 240 TYR ARG GLN SER SER ALA ASN LEU LEU CYS PHE ALA PRO  
SEQRES 9 1 240 ASP LEU ILE ILE ASN GLU GLN ARG MET THR LEU PRO CYS  
SEQRES 10 1 240 MET TYR ASP GLN CYS LYS HIS MET LEU TYR VAL SER SER  
SEQRES 11 1 240 GLU LEU HIS ARG LEU GLN VAL SER TYR GLU GLU TYR LEU  
SEQRES 12 1 240 CYS MET LYS THR LEU LEU LEU LEU SER SER VAL PRO LYS  
SEQRES 13 1 240 ASP GLY LEU LYS SER GLN GLU LEU PHE ASP GLU ILE ARG  
SEQRES 14 1 240 MET THR TYR ILE LYS GLU LEU GLY LYS ALA ILE VAL LYS  
SEQRES 15 1 240 ARG GLU GLY ASN SER SER GLN ASN TRP GLN ARG PHE TYR  
SEQRES 16 1 240 GLN LEU THR LYS LEU LEU ASP SER MET HIS GLU VAL VAL  
SEQRES 17 1 240 GLU ASN LEU LEU ASN TYR CYS PHE GLN THR PHE LEU ASP  
SEQRES 18 1 240 LYS THR MET SER ILE GLU PHE PRO GLU MET LEU ALA GLU  
SEQRES 19 1 240 ILE ILE THR ASN GLN ILE  
ATOM 1 N PRO 1 522 -16.028 23.289 -6.590 1.00 0.53  
ATOM 2 CA PRO 1 522 -14.607 22.883 -6.755 1.00 0.53  
ATOM 3 C PRO 1 522 -13.778 23.929 -6.090 1.00 0.53  
ATOM 4 O PRO 1 522 -13.771 25.067 -6.553 1.00 0.53  
ATOM 5 CB PRO 1 522 -14.354 22.795 -8.259 1.00 0.53  
ATOM 6 CG PRO 1 522 -15.411 23.713 -8.885 1.00 0.53  
ATOM 7 CD PRO 1 522 -16.614 23.612 -7.935 1.00 0.53  
ATOM 8 N ALA 1 523 -13.092 23.572 -4.988 1.00 0.45  
ATOM 9 CA ALA 1 523 -12.249 24.517 -4.317 1.00 0.45  
ATOM 10 C ALA 1 523 -11.040 23.762 -3.879 1.00 0.45  
ATOM 11 O ALA 1 523 -10.754 23.666 -2.687 1.00 0.45  
ATOM 12 CB ALA 1 523 -12.896 25.104 -3.051 1.00 0.45  
ATOM 13 N THR 1 524 -10.294 23.202 -4.846 1.00 0.32  
ATOM 14 CA THR 1 524 -9.142 22.418 -4.509 1.00 0.32  
ATOM 15 C THR 1 524 -8.086 23.314 -3.949 1.00 0.32  
ATOM 16 O THR 1 524 -7.626 23.140 -2.823 1.00 0.32  
ATOM 17 CB THR 1 524 -8.553 21.728 -5.703 1.00 0.32  
ATOM 18 OG1 THR 1 524 -9.511 20.859 -6.289 1.00 0.32  
ATOM 19 CG2 THR 1 524 -7.316 20.931 -5.257 1.00 0.32  
ATOM 20 N LEU 1 525 -7.686 24.309 -4.755 1.00 0.35  
ATOM 21 CA LEU 1 525 -6.691 25.285 -4.414 1.00 0.35  
ATOM 22 C LEU 1 525 -7.181 26.176 -3.307 1.00 0.35  
ATOM 23 O LEU 1 525 -6.374 26.650 -2.509 1.00 0.35  
ATOM 24 CB LEU 1 525 -6.316 26.182 -5.605 1.00 0.35  
ATOM 25 CG LEU 1 525 -5.676 25.395 -6.764 1.00 0.35  
ATOM 26 CD1 LEU 1 525 -5.297 26.322 -7.929 1.00 0.35  
ATOM 27 CD2 LEU 1 525 -4.502 24.534 -6.267 1.00 0.35  
ATOM 28 N PRO 1 526 -8.450 26.471 -3.226 1.00 0.52  
ATOM 29 CA PRO 1 526 -8.883 27.338 -2.161 1.00 0.52  
ATOM 30 C PRO 1 526 -8.844 26.769 -0.776 1.00 0.52  
ATOM 31 O PRO 1 526 -9.013 27.542 0.166 1.00 0.52  
ATOM 32 CB PRO 1 526 -10.267 27.842 -2.564 1.00 0.52  
ATOM 33 CG PRO 1 526 -10.218 27.841 -4.098 1.00 0.52  
ATOM 34 CD PRO 1 526 -9.224 26.723 -4.438 1.00 0.52  
ATOM 35 N GLN 1 527 -8.645 25.450 -0.600 1.00 0.57  
ATOM 36 CA GLN 1 527 -8.683 24.919 0.734 1.00 0.57  
ATOM 37 C GLN 1 527 -7.482 25.412 1.476 1.00 0.57  
ATOM 38 O GLN 1 527 -6.393 25.495 0.914 1.00 0.57  
ATOM 39 CB GLN 1 527 -8.653 23.380 0.770 1.00 0.57

142/208

ATOM	40	CG	GLN 1 527	-9.756	22.711	-0.059	1.00	0.57
ATOM	41	CD	GLN 1 527	-11.110	22.880	0.620	1.00	0.57
ATOM	42	OE1	GLN 1 527	-12.023	22.093	0.375	1.00	0.57
ATOM	43	NE2	GLN 1 527	-11.257	23.918	1.487	1.00	0.57
ATOM	44	N	LEU 1 528	-7.636	25.784	2.763	1.00	0.58
ATOM	45	CA	LEU 1 528	-6.462	26.195	3.479	1.00	0.58
ATOM	46	C	LEU 1 528	-5.801	24.950	3.965	1.00	0.58
ATOM	47	O	LEU 1 528	-6.331	23.854	3.792	1.00	0.58
ATOM	48	CB	LEU 1 528	-6.675	27.159	4.667	1.00	0.58
ATOM	49	CG	LEU 1 528	-7.694	26.722	5.733	1.00	0.58
ATOM	50	CD1	LEU 1 528	-7.801	27.774	6.850	1.00	0.58
ATOM	51	CD2	LEU 1 528	-9.065	26.444	5.109	1.00	0.58
ATOM	52	N	THR 1 529	-4.612	25.079	4.583	1.00	0.58
ATOM	53	CA	THR 1 529	-3.936	23.879	4.963	1.00	0.58
ATOM	54	C	THR 1 529	-4.770	23.095	5.934	1.00	0.58
ATOM	55	O	THR 1 529	-4.788	21.870	5.819	1.00	0.58
ATOM	56	CB	THR 1 529	-2.501	24.061	5.426	1.00	0.58
ATOM	57	OG1	THR 1 529	-1.946	22.797	5.757	1.00	0.58
ATOM	58	CG2	THR 1 529	-2.363	25.038	6.602	1.00	0.58
ATOM	59	N	PRO 1 530	-5.490	23.667	6.870	1.00	0.40
ATOM	60	CA	PRO 1 530	-6.256	22.847	7.763	1.00	0.40
ATOM	61	C	PRO 1 530	-7.366	22.137	7.055	1.00	0.40
ATOM	62	O	PRO 1 530	-7.691	21.014	7.434	1.00	0.40
ATOM	63	CB	PRO 1 530	-6.764	23.777	8.864	1.00	0.40
ATOM	64	CG	PRO 1 530	-5.753	24.936	8.868	1.00	0.40
ATOM	65	CD	PRO 1 530	-5.255	24.995	7.414	1.00	0.40
ATOM	66	N	THR 1 531	-7.983	22.770	6.042	1.00	0.29
ATOM	67	CA	THR 1 531	-9.075	22.121	5.380	1.00	0.29
ATOM	68	C	THR 1 531	-8.576	20.949	4.613	1.00	0.29
ATOM	69	O	THR 1 531	-9.227	19.906	4.578	1.00	0.29
ATOM	70	CB	THR 1 531	-9.836	22.998	4.432	1.00	0.29
ATOM	71	OG1	THR 1 531	-10.469	24.049	5.145	1.00	0.29
ATOM	72	CG2	THR 1 531	-10.891	22.143	3.711	1.00	0.29
ATOM	73	N	LEU 1 532	-7.401	21.081	3.976	1.00	0.43
ATOM	74	CA	LEU 1 532	-6.959	19.997	3.159	1.00	0.43
ATOM	75	C	LEU 1 532	-6.677	18.816	4.031	1.00	0.43
ATOM	76	O	LEU 1 532	-7.015	17.685	3.683	1.00	0.43
ATOM	77	CB	LEU 1 532	-5.747	20.340	2.265	1.00	0.43
ATOM	78	CG	LEU 1 532	-4.353	20.319	2.913	1.00	0.43
ATOM	79	CD1	LEU 1 532	-3.873	18.879	3.165	1.00	0.43
ATOM	80	CD2	LEU 1 532	-3.361	21.138	2.069	1.00	0.43
ATOM	81	N	VAL 1 533	-6.067	19.049	5.209	1.00	0.49
ATOM	82	CA	VAL 1 533	-5.715	17.947	6.056	1.00	0.49
ATOM	83	C	VAL 1 533	-6.944	17.239	6.527	1.00	0.49
ATOM	84	O	VAL 1 533	-6.973	16.010	6.589	1.00	0.49
ATOM	85	CB	VAL 1 533	-4.900	18.342	7.257	1.00	0.49
ATOM	86	CG1	VAL 1 533	-5.708	19.275	8.167	1.00	0.49
ATOM	87	CG2	VAL 1 533	-4.467	17.053	7.963	1.00	0.49
ATOM	88	N	SER 1 534	-7.991	18.003	6.879	1.00	0.55
ATOM	89	CA	SER 1 534	-9.207	17.441	7.387	1.00	0.55
ATOM	90	C	SER 1 534	-9.854	16.647	6.309	1.00	0.55
ATOM	91	O	SER 1 534	-10.263	15.505	6.523	1.00	0.55
ATOM	92	CB	SER 1 534	-10.207	18.537	7.772	1.00	0.55
ATOM	93	OG	SER 1 534	-9.571	19.462	8.638	1.00	0.55
ATOM	94	N	LEU 1 535	-9.927	17.235	5.100	1.00	0.57
ATOM	95	CA	LEU 1 535	-10.614	16.574	4.038	1.00	0.57
ATOM	96	C	LEU 1 535	-9.930	15.269	3.823	1.00	0.57
ATOM	97	O	LEU 1 535	-10.590	14.235	3.815	1.00	0.57
ATOM	98	CB	LEU 1 535	-10.646	17.394	2.728	1.00	0.57
ATOM	99	CG	LEU 1 535	-9.329	17.490	1.931	1.00	0.57
ATOM	100	CD1	LEU 1 535	-9.023	16.194	1.160	1.00	0.57



143/208

ATOM	101	CD2 LEU 1 535	-9.326	18.725	1.017	1.00	0.57
ATOM	102	N LEU 1 536	-8.585	15.266	3.780	1.00	0.36
ATOM	103	CA LEU 1 536	-7.854	14.065	3.497	1.00	0.36
ATOM	104	C LEU 1 536	-8.202	13.040	4.523	1.00	0.36
ATOM	105	O LEU 1 536	-8.454	11.880	4.202	1.00	0.36
ATOM	106	CB LEU 1 536	-6.330	14.267	3.528	1.00	0.36
ATOM	107	CG LEU 1 536	-5.795	15.178	2.406	1.00	0.36
ATOM	108	CD1 LEU 1 536	-4.268	15.327	2.499	1.00	0.36
ATOM	109	CD2 LEU 1 536	-6.252	14.697	1.019	1.00	0.36
ATOM	110	N GLU 1 537	-8.286	13.471	5.789	1.00	0.30
ATOM	111	CA GLU 1 537	-8.523	12.577	6.880	1.00	0.30
ATOM	112	C GLU 1 537	-9.791	11.829	6.603	1.00	0.30
ATOM	113	O GLU 1 537	-9.855	10.616	6.795	1.00	0.30
ATOM	114	CB GLU 1 537	-8.758	13.357	8.187	1.00	0.30
ATOM	115	CG GLU 1 537	-7.578	14.236	8.617	1.00	0.30
ATOM	116	CD GLU 1 537	-6.858	13.565	9.776	1.00	0.30
ATOM	117	OE1 GLU 1 537	-7.484	12.693	10.434	1.00	0.30
ATOM	118	OE2 GLU 1 537	-5.676	13.924	10.026	1.00	0.30
ATOM	119	N VAL 1 538	-10.840	12.536	6.138	1.00	0.42
ATOM	120	CA VAL 1 538	-12.105	11.892	5.920	1.00	0.42
ATOM	121	C VAL 1 538	-12.006	10.913	4.790	1.00	0.42
ATOM	122	O VAL 1 538	-12.638	9.860	4.833	1.00	0.42
ATOM	123	CB VAL 1 538	-13.248	12.823	5.614	1.00	0.42
ATOM	124	CG1 VAL 1 538	-13.139	13.335	4.172	1.00	0.42
ATOM	125	CG2 VAL 1 538	-14.561	12.066	5.876	1.00	0.42
ATOM	126	N ILE 1 539	-11.197	11.220	3.755	1.00	0.45
ATOM	127	CA ILE 1 539	-11.156	10.375	2.592	1.00	0.45
ATOM	128	C ILE 1 539	-10.713	9.001	2.955	1.00	0.45
ATOM	129	O ILE 1 539	-11.189	8.053	2.331	1.00	0.45
ATOM	130	CB ILE 1 539	-10.184	10.755	1.482	1.00	0.45
ATOM	131	CG1 ILE 1 539	-10.455	12.113	0.848	1.00	0.45
ATOM	132	CG2 ILE 1 539	-10.253	9.685	0.381	1.00	0.45
ATOM	133	CD1 ILE 1 539	-9.752	13.325	1.403	1.00	0.45
ATOM	134	N GLU 1 540	-9.802	8.870	3.950	1.00	0.40
ATOM	135	CA GLU 1 540	-9.162	7.620	4.284	1.00	0.40
ATOM	136	C GLU 1 540	-10.111	6.470	4.207	1.00	0.40
ATOM	137	O GLU 1 540	-11.258	6.517	4.643	1.00	0.40
ATOM	138	CB GLU 1 540	-8.435	7.601	5.638	1.00	0.40
ATOM	139	CG GLU 1 540	-7.105	8.365	5.615	1.00	0.40
ATOM	140	CD GLU 1 540	-6.012	7.490	5.001	1.00	0.40
ATOM	141	OE1 GLU 1 540	-5.911	7.472	3.745	1.00	0.40
ATOM	142	OE2 GLU 1 540	-5.264	6.835	5.776	1.00	0.40
ATOM	143	N PRO 1 541	-9.627	5.476	3.519	1.00	0.41
ATOM	144	CA PRO 1 541	-10.361	4.273	3.259	1.00	0.41
ATOM	145	C PRO 1 541	-10.454	3.492	4.522	1.00	0.41
ATOM	146	O PRO 1 541	-9.655	3.728	5.426	1.00	0.41
ATOM	147	CB PRO 1 541	-9.593	3.541	2.157	1.00	0.41
ATOM	148	CG PRO 1 541	-8.192	4.181	2.174	1.00	0.41
ATOM	149	CD PRO 1 541	-8.451	5.609	2.679	1.00	0.41
ATOM	150	N GLU 1 542	-11.438	2.578	4.608	1.00	0.55
ATOM	151	CA GLU 1 542	-11.611	1.777	5.784	1.00	0.55
ATOM	152	C GLU 1 542	-10.650	0.635	5.706	1.00	0.55
ATOM	153	O GLU 1 542	-10.161	0.290	4.632	1.00	0.55
ATOM	154	CB GLU 1 542	-13.021	1.175	5.913	1.00	0.55
ATOM	155	CG GLU 1 542	-13.381	0.217	4.774	1.00	0.55
ATOM	156	CD GLU 1 542	-13.569	1.035	3.503	1.00	0.55
ATOM	157	OE1 GLU 1 542	-13.850	2.258	3.621	1.00	0.55
ATOM	158	OE2 GLU 1 542	-13.435	0.446	2.398	1.00	0.55
ATOM	159	N VAL 1 543	-10.345	0.019	6.866	1.00	0.62
ATOM	160	CA VAL 1 543	-9.445	-1.094	6.867	1.00	0.62
ATOM	161	C VAL 1 543	-10.277	-2.304	6.592	1.00	0.62

144/208

ATOM	162	O	VAL 1 543	-11.280	-2.557	7.257	1.00	0.62
ATOM	163	CB	VAL 1 543	-8.728	-1.292	8.174	1.00	0.62
ATOM	164	CG1	VAL 1 543	-7.825	-0.070	8.417	1.00	0.62
ATOM	165	CG2	VAL 1 543	-9.761	-1.519	9.291	1.00	0.62
ATOM	166	N	LEU 1 544	-9.879	-3.078	5.568	1.00	0.55
ATOM	167	CA	LEU 1 544	-10.688	-4.183	5.156	1.00	0.55
ATOM	168	C	LEU 1 544	-10.086	-5.420	5.775	1.00	0.55
ATOM	169	O	LEU 1 544	-8.950	-5.384	6.242	1.00	0.55
ATOM	170	CB	LEU 1 544	-10.673	-4.279	3.619	1.00	0.55
ATOM	171	CG	LEU 1 544	-11.936	-4.888	2.996	1.00	0.55
ATOM	172	CD1	LEU 1 544	-12.128	-6.370	3.323	1.00	0.55
ATOM	173	CD2	LEU 1 544	-13.153	-4.023	3.367	1.00	0.55
ATOM	174	N	TYR 1 545	-10.839	-6.543	5.819	1.00	0.30
ATOM	175	CA	TYR 1 545	-10.348	-7.774	6.387	1.00	0.30
ATOM	176	C	TYR 1 545	-10.140	-8.792	5.312	1.00	0.30
ATOM	177	O	TYR 1 545	-10.716	-8.721	4.228	1.00	0.30
ATOM	178	CB	TYR 1 545	-11.290	-8.448	7.403	1.00	0.30
ATOM	179	CG	TYR 1 545	-11.220	-7.730	8.701	1.00	0.30
ATOM	180	CD1	TYR 1 545	-11.929	-6.571	8.912	1.00	0.30
ATOM	181	CD2	TYR 1 545	-10.443	-8.236	9.719	1.00	0.30
ATOM	182	CE1	TYR 1 545	-11.858	-5.921	10.122	1.00	0.30
ATOM	183	CE2	TYR 1 545	-10.367	-7.590	10.930	1.00	0.30
ATOM	184	CZ	TYR 1 545	-11.075	-6.429	11.131	1.00	0.30
ATOM	185	OH	TYR 1 545	-11.002	-5.762	12.372	1.00	0.30
ATOM	186	N	ALA 1 546	-9.278	-9.785	5.615	1.00	0.14
ATOM	187	CA	ALA 1 546	-8.982	-10.841	4.694	1.00	0.14
ATOM	188	C	ALA 1 546	-10.145	-11.770	4.684	1.00	0.14
ATOM	189	O	ALA 1 546	-10.982	-11.740	5.587	1.00	0.14
ATOM	190	CB	ALA 1 546	-7.738	-11.662	5.083	1.00	0.14
ATOM	191	N	GLY 1 547	-10.216	-12.613	3.630	1.00	0.34
ATOM	192	CA	GLY 1 547	-11.275	-13.568	3.511	1.00	0.34
ATOM	193	C	GLY 1 547	-11.244	-14.321	4.785	1.00	0.34
ATOM	194	O	GLY 1 547	-10.171	-14.684	5.265	1.00	0.34
ATOM	195	N	TYR 1 548	-12.449	-14.541	5.345	1.00	0.58
ATOM	196	CA	TYR 1 548	-12.684	-15.135	6.626	1.00	0.58
ATOM	197	C	TYR 1 548	-11.775	-16.315	6.726	1.00	0.58
ATOM	198	O	TYR 1 548	-11.435	-16.897	5.699	1.00	0.58
ATOM	199	CB	TYR 1 548	-14.140	-15.607	6.753	1.00	0.58
ATOM	200	CG	TYR 1 548	-14.519	-15.633	8.188	1.00	0.58
ATOM	201	CD1	TYR 1 548	-14.196	-16.688	9.009	1.00	0.58
ATOM	202	CD2	TYR 1 548	-15.222	-14.569	8.705	1.00	0.58
ATOM	203	CE1	TYR 1 548	-14.573	-16.672	10.332	1.00	0.58
ATOM	204	CE2	TYR 1 548	-15.600	-14.550	10.024	1.00	0.58
ATOM	205	CZ	TYR 1 548	-15.276	-15.605	10.840	1.00	0.58
ATOM	206	OH	TYR 1 548	-15.663	-15.589	12.197	1.00	0.58
ATOM	207	N	ASP 1 549	-11.358	-16.651	7.969	1.00	0.54
ATOM	208	CA	ASP 1 549	-10.379	-17.663	8.288	1.00	0.54
ATOM	209	C	ASP 1 549	-10.510	-18.822	7.361	1.00	0.54
ATOM	210	O	ASP 1 549	-11.474	-19.585	7.410	1.00	0.54
ATOM	211	CB	ASP 1 549	-10.504	-18.197	9.724	1.00	0.54
ATOM	212	CG	ASP 1 549	-9.269	-19.029	10.034	1.00	0.54
ATOM	213	OD1	ASP 1 549	-8.168	-18.659	9.548	1.00	0.54
ATOM	214	OD2	ASP 1 549	-9.412	-20.054	10.752	1.00	0.54
ATOM	215	N	SER 1 550	-9.516	-18.955	6.468	1.00	0.52
ATOM	216	CA	SER 1 550	-9.517	-19.997	5.491	1.00	0.52
ATOM	217	C	SER 1 550	-8.795	-21.150	6.105	1.00	0.52
ATOM	218	O	SER 1 550	-9.384	-21.939	6.843	1.00	0.52
ATOM	219	CB	SER 1 550	-8.791	-19.574	4.201	1.00	0.52
ATOM	220	OG	SER 1 550	-9.124	-20.448	3.134	1.00	0.52
ATOM	221	N	SER 1 551	-7.485	-21.273	5.821	1.00	0.82
ATOM	222	CA	SER 1 551	-6.734	-22.361	6.369	1.00	0.82

145/208

ATOM	223	C	SER	1 551	-5.454	-21.817	6.918	1.00	0.82
ATOM	224	O	SER	1 551	-4.927	-20.803	6.454	1.00	0.82
ATOM	225	CB	SER	1 551	-6.370	-23.444	5.341	1.00	0.82
ATOM	226	OG	SER	1 551	-5.631	-24.481	5.968	1.00	0.82
ATOM	227	N	VAL	1 552	-4.895	-22.551	7.898	1.00	1.25
ATOM	228	CA	VAL	1 552	-3.740	-22.163	8.639	1.00	1.25
ATOM	229	C	VAL	1 552	-2.505	-22.265	7.824	1.00	1.25
ATOM	230	O	VAL	1 552	-2.276	-21.246	7.175	1.00	1.25
ATOM	231	CB	VAL	1 552	-3.665	-22.788	10.017	1.00	1.25
ATOM	232	CG1	VAL	1 552	-4.317	-24.185	10.023	1.00	1.25
ATOM	233	CG2	VAL	1 552	-2.212	-22.736	10.521	1.00	1.25
ATOM	234	N	PRO	1 553	-1.656	-23.294	7.852	1.00	1.24
ATOM	235	CA	PRO	1 553	-0.494	-23.299	7.002	1.00	1.24
ATOM	236	C	PRO	1 553	-1.006	-23.041	5.633	1.00	1.24
ATOM	237	O	PRO	1 553	-1.720	-23.877	5.077	1.00	1.24
ATOM	238	CB	PRO	1 553	0.109	-24.700	7.080	1.00	1.24
ATOM	239	CG	PRO	1 553	-0.775	-25.455	8.087	1.00	1.24
ATOM	240	CD	PRO	1 553	-2.092	-24.663	8.072	1.00	1.24
ATOM	241	N	ASP	1 554	-0.651	-21.875	5.086	1.00	0.74
ATOM	242	CA	ASP	1 554	-1.205	-21.454	3.852	1.00	0.74
ATOM	243	C	ASP	1 554	-0.299	-22.024	2.812	1.00	0.74
ATOM	244	O	ASP	1 554	0.819	-22.433	3.122	1.00	0.74
ATOM	245	CB	ASP	1 554	-1.198	-19.915	3.772	1.00	0.74
ATOM	246	CG	ASP	1 554	-2.288	-19.460	2.829	1.00	0.74
ATOM	247	OD1	ASP	1 554	-2.369	-20.056	1.729	1.00	0.74
ATOM	248	OD2	ASP	1 554	-3.047	-18.523	3.186	1.00	0.74
ATOM	249	N	SER	1 555	-0.788	-22.127	1.566	1.00	0.52
ATOM	250	CA	SER	1 555	0.017	-22.585	0.482	1.00	0.52
ATOM	251	C	SER	1 555	0.411	-21.346	-0.245	1.00	0.52
ATOM	252	O	SER	1 555	-0.037	-20.255	0.102	1.00	0.52
ATOM	253	CB	SER	1 555	-0.745	-23.477	-0.511	1.00	0.52
ATOM	254	OG	SER	1 555	0.119	-23.884	-1.560	1.00	0.52
ATOM	255	N	THR	1 556	1.283	-21.469	-1.261	1.00	0.67
ATOM	256	CA	THR	1 556	1.635	-20.279	-1.968	1.00	0.67
ATOM	257	C	THR	1 556	0.398	-19.746	-2.613	1.00	0.67
ATOM	258	O	THR	1 556	0.010	-18.605	-2.377	1.00	0.67
ATOM	259	CB	THR	1 556	2.656	-20.525	-3.041	1.00	0.67
ATOM	260	OG1	THR	1 556	2.149	-21.432	-4.009	1.00	0.67
ATOM	261	CG2	THR	1 556	3.923	-21.104	-2.388	1.00	0.67
ATOM	262	N	TRP	1 557	-0.301	-20.612	-3.368	1.00	0.70
ATOM	263	CA	TRP	1 557	-1.440	-20.245	-4.162	1.00	0.70
ATOM	264	C	TRP	1 557	-2.526	-19.719	-3.283	1.00	0.70
ATOM	265	O	TRP	1 557	-3.155	-18.706	-3.583	1.00	0.70
ATOM	266	CB	TRP	1 557	-1.997	-21.469	-4.910	1.00	0.70
ATOM	267	CG	TRP	1 557	-3.196	-21.218	-5.788	1.00	0.70
ATOM	268	CD1	TRP	1 557	-4.524	-21.206	-5.474	1.00	0.70
ATOM	269	CD2	TRP	1 557	-3.109	-20.981	-7.202	1.00	0.70
ATOM	270	NE1	TRP	1 557	-5.270	-20.973	-6.604	1.00	0.70
ATOM	271	CE2	TRP	1 557	-4.412	-20.834	-7.676	1.00	0.70
ATOM	272	CE3	TRP	1 557	-2.032	-20.898	-8.037	1.00	0.70
ATOM	273	CZ2	TRP	1 557	-4.659	-20.602	-8.999	1.00	0.70
ATOM	274	CZ3	TRP	1 557	-2.284	-20.658	-9.369	1.00	0.70
ATOM	275	CH2	TRP	1 557	-3.572	-20.513	-9.841	1.00	0.70
ATOM	276	N	ARG	1 558	-2.761	-20.403	-2.156	1.00	0.62
ATOM	277	CA	ARG	1 558	-3.840	-20.090	-1.271	1.00	0.62
ATOM	278	C	ARG	1 558	-3.595	-18.732	-0.674	1.00	0.62
ATOM	279	O	ARG	1 558	-4.516	-17.927	-0.531	1.00	0.62
ATOM	280	CB	ARG	1 558	-3.922	-21.191	-0.201	1.00	0.62
ATOM	281	CG	ARG	1 558	-5.283	-21.459	0.429	1.00	0.62
ATOM	282	CD	ARG	1 558	-5.232	-22.749	1.249	1.00	0.62
ATOM	283	NE	ARG	1 558	-6.617	-23.150	1.607	1.00	0.62

146/208

ATOM	284	CZ ARG 1 558	-7.220	-22.547	2.666	1.00	0.62
ATOM	285	NH1 ARG 1 558	-6.619	-21.461	3.233	1.00	0.62
ATOM	286	NH2 ARG 1 558	-8.394	-23.043	3.159	1.00	0.62
ATOM	287	N ILE 1 559	-2.328	-18.441	-0.319	1.00	0.68
ATOM	288	CA ILE 1 559	-1.993	-17.195	0.305	1.00	0.68
ATOM	289	C ILE 1 559	-2.140	-16.110	-0.727	1.00	0.68
ATOM	290	O ILE 1 559	-2.665	-15.035	-0.434	1.00	0.68
ATOM	291	CB ILE 1 559	-0.591	-17.232	0.870	1.00	0.68
ATOM	292	CG1 ILE 1 559	-0.472	-16.357	2.130	1.00	0.68
ATOM	293	CG2 ILE 1 559	0.421	-16.889	-0.235	1.00	0.68
ATOM	294	CD1 ILE 1 559	-0.907	-14.910	1.959	1.00	0.68
ATOM	295	N MET 1 560	-1.714	-16.347	-1.989	1.00	0.55
ATOM	296	CA MET 1 560	-1.890	-15.270	-2.919	1.00	0.55
ATOM	297	C MET 1 560	-3.342	-15.050	-3.136	1.00	0.55
ATOM	298	O MET 1 560	-3.758	-13.942	-3.463	1.00	0.55
ATOM	299	CB MET 1 560	-1.182	-15.317	-4.293	1.00	0.55
ATOM	300	CG MET 1 560	-1.169	-16.608	-5.100	1.00	0.55
ATOM	301	SD MET 1 560	0.410	-17.486	-4.965	1.00	0.55
ATOM	302	CE MET 1 560	1.404	-15.974	-5.136	1.00	0.55
ATOM	303	N THR 1 561	-4.159	-16.104	-2.982	1.00	0.35
ATOM	304	CA THR 1 561	-5.567	-15.934	-3.165	1.00	0.35
ATOM	305	C THR 1 561	-6.036	-14.922	-2.169	1.00	0.35
ATOM	306	O THR 1 561	-6.763	-13.993	-2.519	1.00	0.35
ATOM	307	CB THR 1 561	-6.332	-17.202	-2.922	1.00	0.35
ATOM	308	OG1 THR 1 561	-5.891	-18.216	-3.812	1.00	0.35
ATOM	309	CG2 THR 1 561	-7.829	-16.923	-3.138	1.00	0.35
ATOM	310	N THR 1 562	-5.616	-15.058	-0.897	1.00	0.42
ATOM	311	CA THR 1 562	-6.088	-14.116	0.072	1.00	0.42
ATOM	312	C THR 1 562	-5.571	-12.755	-0.281	1.00	0.42
ATOM	313	O THR 1 562	-6.331	-11.790	-0.291	1.00	0.42
ATOM	314	CB THR 1 562	-5.697	-14.444	1.491	1.00	0.42
ATOM	315	OG1 THR 1 562	-6.420	-13.617	2.390	1.00	0.42
ATOM	316	CG2 THR 1 562	-4.189	-14.233	1.693	1.00	0.42
ATOM	317	N LEU 1 563	-4.274	-12.628	-0.630	1.00	0.48
ATOM	318	CA LEU 1 563	-3.812	-11.295	-0.893	1.00	0.48
ATOM	319	C LEU 1 563	-4.507	-10.730	-2.086	1.00	0.48
ATOM	320	O LEU 1 563	-4.833	-9.546	-2.102	1.00	0.48
ATOM	321	CB LEU 1 563	-2.312	-11.103	-1.184	1.00	0.48
ATOM	322	CG LEU 1 563	-1.359	-11.510	-0.054	1.00	0.48
ATOM	323	CD1 LEU 1 563	-0.892	-12.955	-0.232	1.00	0.48
ATOM	324	CD2 LEU 1 563	-0.222	-10.500	0.130	1.00	0.48
ATOM	325	N ASN 1 564	-4.738	-11.543	-3.133	1.00	0.45
ATOM	326	CA ASN 1 564	-5.334	-10.982	-4.308	1.00	0.45
ATOM	327	C ASN 1 564	-6.723	-10.530	-3.997	1.00	0.45
ATOM	328	O ASN 1 564	-7.157	-9.479	-4.468	1.00	0.45
ATOM	329	CB ASN 1 564	-5.342	-11.908	-5.547	1.00	0.45
ATOM	330	CG ASN 1 564	-6.153	-13.175	-5.323	1.00	0.45
ATOM	331	OD1 ASN 1 564	-7.341	-13.161	-5.012	1.00	0.45
ATOM	332	ND2 ASN 1 564	-5.478	-14.336	-5.537	1.00	0.45
ATOM	333	N MET 1 565	-7.457	-11.302	-3.178	1.00	0.57
ATOM	334	CA MET 1 565	-8.801	-10.924	-2.869	1.00	0.57
ATOM	335	C MET 1 565	-8.751	-9.606	-2.162	1.00	0.57
ATOM	336	O MET 1 565	-9.518	-8.697	-2.478	1.00	0.57
ATOM	337	CB MET 1 565	-9.497	-11.922	-1.926	1.00	0.57
ATOM	338	CG MET 1 565	-9.752	-13.294	-2.552	1.00	0.57
ATOM	339	SD MET 1 565	-11.044	-13.308	-3.832	1.00	0.57
ATOM	340	CE MET 1 565	-12.418	-13.115	-2.659	1.00	0.57
ATOM	341	N LEU 1 566	-7.810	-9.457	-1.207	1.00	0.62
ATOM	342	CA LEU 1 566	-7.746	-8.253	-0.424	1.00	0.62
ATOM	343	C LEU 1 566	-7.560	-7.082	-1.330	1.00	0.62
ATOM	344	O LEU 1 566	-8.369	-6.156	-1.346	1.00	0.62

147/208

ATOM	345	CB	LEU	1 566	-6.494	-8.156	0.468	1.00	0.62
ATOM	346	CG	LEU	1 566	-6.327	-9.185	1.593	1.00	0.62
ATOM	347	CD1	LEU	1 566	-5.025	-8.912	2.356	1.00	0.62
ATOM	348	CD2	LEU	1 566	-7.526	-9.206	2.544	1.00	0.62
ATOM	349	N	GLY	1 567	-6.508	-7.138	-2.163	1.00	0.32
ATOM	350	CA	GLY	1 567	-6.125	-6.004	-2.951	1.00	0.32
ATOM	351	C	GLY	1 567	-7.264	-5.586	-3.817	1.00	0.32
ATOM	352	O	GLY	1 567	-7.508	-4.391	-3.993	1.00	0.32
ATOM	353	N	GLY	1 568	-7.985	-6.561	-4.396	1.00	0.15
ATOM	354	CA	GLY	1 568	-9.067	-6.225	-5.273	1.00	0.15
ATOM	355	C	GLY	1 568	-10.115	-5.496	-4.497	1.00	0.15
ATOM	356	O	GLY	1 568	-10.693	-4.518	-4.966	1.00	0.15
ATOM	357	N	ARG	1 569	-10.416	-5.965	-3.279	1.00	0.29
ATOM	358	CA	ARG	1 569	-11.425	-5.314	-2.501	1.00	0.29
ATOM	359	C	ARG	1 569	-10.953	-3.935	-2.166	1.00	0.29
ATOM	360	O	ARG	1 569	-11.705	-2.966	-2.267	1.00	0.29
ATOM	361	CB	ARG	1 569	-11.706	-6.079	-1.199	1.00	0.29
ATOM	362	CG	ARG	1 569	-12.507	-7.367	-1.421	1.00	0.29
ATOM	363	CD	ARG	1 569	-12.352	-8.380	-0.287	1.00	0.29
ATOM	364	NE	ARG	1 569	-11.653	-7.671	0.816	1.00	0.29
ATOM	365	CZ	ARG	1 569	-10.466	-8.155	1.286	1.00	0.29
ATOM	366	NH1	ARG	1 569	-10.029	-9.385	0.889	1.00	0.29
ATOM	367	NH2	ARG	1 569	-9.718	-7.402	2.145	1.00	0.29
ATOM	368	N	GLN	1 570	-9.673	-3.797	-1.780	1.00	0.39
ATOM	369	CA	GLN	1 570	-9.166	-2.514	-1.394	1.00	0.39
ATOM	370	C	GLN	1 570	-9.169	-1.588	-2.572	1.00	0.39
ATOM	371	O	GLN	1 570	-9.385	-0.387	-2.413	1.00	0.39
ATOM	372	CB	GLN	1 570	-7.741	-2.554	-0.795	1.00	0.39
ATOM	373	CG	GLN	1 570	-7.646	-3.202	0.597	1.00	0.39
ATOM	374	CD	GLN	1 570	-6.226	-3.075	1.130	1.00	0.39
ATOM	375	OE1	GLN	1 570	-5.984	-2.404	2.132	1.00	0.39
ATOM	376	NE2	GLN	1 570	-5.255	-3.728	0.438	1.00	0.39
ATOM	377	N	VAL	1 571	-8.955	-2.114	-3.796	1.00	0.43
ATOM	378	CA	VAL	1 571	-8.860	-1.235	-4.928	1.00	0.43
ATOM	379	C	VAL	1 571	-10.133	-0.455	-5.052	1.00	0.43
ATOM	380	O	VAL	1 571	-10.111	0.714	-5.429	1.00	0.43
ATOM	381	CB	VAL	1 571	-8.624	-1.921	-6.244	1.00	0.43
ATOM	382	CG1	VAL	1 571	-9.932	-2.569	-6.721	1.00	0.43
ATOM	383	CG2	VAL	1 571	-8.070	-0.884	-7.233	1.00	0.43
ATOM	384	N	ILE	1 572	-11.286	-1.072	-4.735	1.00	0.36
ATOM	385	CA	ILE	1 572	-12.526	-0.363	-4.890	1.00	0.36
ATOM	386	C	ILE	1 572	-12.559	0.843	-3.992	1.00	0.36
ATOM	387	O	ILE	1 572	-12.992	1.917	-4.407	1.00	0.36
ATOM	388	CB	ILE	1 572	-13.750	-1.197	-4.607	1.00	0.36
ATOM	389	CG1	ILE	1 572	-15.002	-0.501	-5.160	1.00	0.36
ATOM	390	CG2	ILE	1 572	-13.842	-1.473	-3.099	1.00	0.36
ATOM	391	CD1	ILE	1 572	-16.238	-1.400	-5.177	1.00	0.36
ATOM	392	N	ALA	1 573	-12.095	0.712	-2.737	1.00	0.18
ATOM	393	CA	ALA	1 573	-12.146	1.810	-1.808	1.00	0.18
ATOM	394	C	ALA	1 573	-11.235	2.896	-2.281	1.00	0.18
ATOM	395	O	ALA	1 573	-11.529	4.080	-2.128	1.00	0.18
ATOM	396	CB	ALA	1 573	-11.693	1.413	-0.393	1.00	0.18
ATOM	397	N	ALA	1 574	-10.102	2.505	-2.886	1.00	0.10
ATOM	398	CA	ALA	1 574	-9.103	3.437	-3.319	1.00	0.10
ATOM	399	C	ALA	1 574	-9.701	4.372	-4.319	1.00	0.10
ATOM	400	O	ALA	1 574	-9.374	5.557	-4.339	1.00	0.10
ATOM	401	CB	ALA	1 574	-7.897	2.757	-3.989	1.00	0.10
ATOM	402	N	VAL	1 575	-10.594	3.861	-5.186	1.00	0.13
ATOM	403	CA	VAL	1 575	-11.188	4.703	-6.181	1.00	0.13
ATOM	404	C	VAL	1 575	-11.953	5.790	-5.492	1.00	0.13
ATOM	405	O	VAL	1 575	-11.871	6.956	-5.876	1.00	0.13

148/208

ATOM	406	CB	VAL 1 575	-12.150	3.966	-7.066	1.00	0.13
ATOM	407	CG1	VAL 1 575	-12.748	4.963	-8.073	1.00	0.13
ATOM	408	CG2	VAL 1 575	-11.410	2.787	-7.721	1.00	0.13
ATOM	409	N	LYS 1 576	-12.708	5.434	-4.434	1.00	0.27
ATOM	410	CA	LYS 1 576	-13.506	6.397	-3.726	1.00	0.27
ATOM	411	C	LYS 1 576	-12.598	7.442	-3.153	1.00	0.27
ATOM	412	O	LYS 1 576	-12.867	8.637	-3.244	1.00	0.27
ATOM	413	CB	LYS 1 576	-14.254	5.786	-2.530	1.00	0.27
ATOM	414	CG	LYS 1 576	-15.304	4.736	-2.900	1.00	0.27
ATOM	415	CD	LYS 1 576	-15.768	3.912	-1.697	1.00	0.27
ATOM	416	CE	LYS 1 576	-16.829	2.861	-2.034	1.00	0.27
ATOM	417	NZ	LYS 1 576	-18.125	3.522	-2.303	1.00	0.27
ATOM	418	N	TRP 1 577	-11.490	6.999	-2.532	1.00	0.34
ATOM	419	CA	TRP 1 577	-10.507	7.863	-1.941	1.00	0.34
ATOM	420	C	TRP 1 577	-9.883	8.746	-2.973	1.00	0.34
ATOM	421	O	TRP 1 577	-9.815	9.963	-2.800	1.00	0.34
ATOM	422	CB	TRP 1 577	-9.498	7.010	-1.129	1.00	0.34
ATOM	423	CG	TRP 1 577	-8.000	7.274	-1.103	1.00	0.34
ATOM	424	CD1	TRP 1 577	-7.050	6.298	-1.185	1.00	0.34
ATOM	425	CD2	TRP 1 577	-7.281	8.520	-1.094	1.00	0.34
ATOM	426	NE1	TRP 1 577	-5.795	6.847	-1.172	1.00	0.34
ATOM	427	CE2	TRP 1 577	-5.919	8.214	-1.134	1.00	0.34
ATOM	428	CE3	TRP 1 577	-7.705	9.813	-1.069	1.00	0.34
ATOM	429	CZ2	TRP 1 577	-4.970	9.194	-1.145	1.00	0.34
ATOM	430	CZ3	TRP 1 577	-6.746	10.801	-1.073	1.00	0.34
ATOM	431	CH2	TRP 1 577	-5.403	10.498	-1.108	1.00	0.34
ATOM	432	N	ALA 1 578	-9.500	8.184	-4.123	1.00	0.38
ATOM	433	CA	ALA 1 578	-8.844	8.981	-5.119	1.00	0.38
ATOM	434	C	ALA 1 578	-9.740	10.111	-5.529	1.00	0.38
ATOM	435	O	ALA 1 578	-9.284	11.234	-5.737	1.00	0.38
ATOM	436	CB	ALA 1 578	-8.500	8.174	-6.382	1.00	0.38
ATOM	437	N	LYS 1 579	-11.054	9.855	-5.618	1.00	0.46
ATOM	438	CA	LYS 1 579	-11.975	10.855	-6.081	1.00	0.46
ATOM	439	C	LYS 1 579	-11.960	12.028	-5.153	1.00	0.46
ATOM	440	O	LYS 1 579	-12.185	13.160	-5.567	1.00	0.46
ATOM	441	CB	LYS 1 579	-13.420	10.341	-6.175	1.00	0.46
ATOM	442	CG	LYS 1 579	-13.604	9.242	-7.225	1.00	0.46
ATOM	443	CD	LYS 1 579	-13.276	9.676	-8.658	1.00	0.46
ATOM	444	CE	LYS 1 579	-14.392	10.474	-9.336	1.00	0.46
ATOM	445	NZ	LYS 1 579	-14.077	10.676	-10.769	1.00	0.46
ATOM	446	N	ALA 1 580	-11.758	11.774	-3.855	1.00	0.43
ATOM	447	CA	ALA 1 580	-11.760	12.785	-2.845	1.00	0.43
ATOM	448	C	ALA 1 580	-10.472	13.579	-2.782	1.00	0.43
ATOM	449	O	ALA 1 580	-10.416	14.609	-2.111	1.00	0.43
ATOM	450	CB	ALA 1 580	-12.158	12.208	-1.493	1.00	0.43
ATOM	451	N	ILE 1 581	-9.379	13.106	-3.418	1.00	0.38
ATOM	452	CA	ILE 1 581	-8.121	13.804	-3.321	1.00	0.38
ATOM	453	C	ILE 1 581	-8.170	15.059	-4.148	1.00	0.38
ATOM	454	O	ILE 1 581	-8.457	15.055	-5.344	1.00	0.38
ATOM	455	CB	ILE 1 581	-6.970	12.914	-3.708	1.00	0.38
ATOM	456	CG1	ILE 1 581	-5.622	13.452	-3.247	1.00	0.38
ATOM	457	CG2	ILE 1 581	-7.005	12.663	-5.211	1.00	0.38
ATOM	458	CD1	ILE 1 581	-4.559	12.380	-3.445	1.00	0.38
ATOM	459	N	PRO 1 582	-7.861	16.159	-3.513	1.00	0.28
ATOM	460	CA	PRO 1 582	-8.000	17.439	-4.147	1.00	0.28
ATOM	461	C	PRO 1 582	-7.240	17.551	-5.426	1.00	0.28
ATOM	462	O	PRO 1 582	-6.035	17.309	-5.439	1.00	0.28
ATOM	463	CB	PRO 1 582	-7.651	18.469	-3.077	1.00	0.28
ATOM	464	CG	PRO 1 582	-8.048	17.760	-1.764	1.00	0.28
ATOM	465	CD	PRO 1 582	-7.884	16.257	-2.063	1.00	0.28
ATOM	466	N	GLY 1 583	-7.948	17.938	-6.507	1.00	0.17

149/208

ATOM	467	CA	GLY 1 583	-7.365	18.131	-7.802	1.00	0.17
ATOM	468	C	GLY 1 583	-7.628	16.926	-8.654	1.00	0.17
ATOM	469	O	GLY 1 583	-7.624	17.002	-9.880	1.00	0.17
ATOM	470	N	PHE 1 584	-7.905	15.780	-8.015	1.00	0.34
ATOM	471	CA	PHE 1 584	-8.062	14.534	-8.710	1.00	0.34
ATOM	472	C	PHE 1 584	-9.230	14.603	-9.654	1.00	0.34
ATOM	473	O	PHE 1 584	-9.114	14.236	-10.823	1.00	0.34
ATOM	474	CB	PHE 1 584	-8.349	13.418	-7.697	1.00	0.34
ATOM	475	CG	PHE 1 584	-7.943	12.078	-8.200	1.00	0.34
ATOM	476	CD1	PHE 1 584	-6.610	11.776	-8.364	1.00	0.34
ATOM	477	CD2	PHE 1 584	-8.882	11.106	-8.446	1.00	0.34
ATOM	478	CE1	PHE 1 584	-6.221	10.535	-8.807	1.00	0.34
ATOM	479	CE2	PHE 1 584	-8.498	9.865	-8.885	1.00	0.34
ATOM	480	CZ	PHE 1 584	-7.168	9.577	-9.072	1.00	0.34
ATOM	481	N	ARG 1 585	-10.384	15.099	-9.174	1.00	0.46
ATOM	482	CA	ARG 1 585	-11.600	15.107	-9.947	1.00	0.46
ATOM	483	C	ARG 1 585	-11.539	16.089	-11.077	1.00	0.46
ATOM	484	O	ARG 1 585	-12.288	15.959	-12.041	1.00	0.46
ATOM	485	CB	ARG 1 585	-12.877	15.408	-9.147	1.00	0.46
ATOM	486	CG	ARG 1 585	-12.958	16.807	-8.540	1.00	0.46
ATOM	487	CD	ARG 1 585	-14.368	17.134	-8.044	1.00	0.46
ATOM	488	NE	ARG 1 585	-15.276	17.029	-9.224	1.00	0.46
ATOM	489	CZ	ARG 1 585	-16.560	16.590	-9.074	1.00	0.46
ATOM	490	NH1	ARG 1 585	-17.032	16.261	-7.836	1.00	0.46
ATOM	491	NH2	ARG 1 585	-17.373	16.476	-10.166	1.00	0.46
ATOM	492	N	ASN 1 586	-10.706	17.139	-10.973	1.00	0.45
ATOM	493	CA	ASN 1 586	-10.634	18.120	-12.021	1.00	0.45
ATOM	494	C	ASN 1 586	-10.111	17.463	-13.259	1.00	0.45
ATOM	495	O	ASN 1 586	-10.475	17.821	-14.380	1.00	0.45
ATOM	496	CB	ASN 1 586	-9.703	19.293	-11.678	1.00	0.45
ATOM	497	CG	ASN 1 586	-10.385	20.101	-10.584	1.00	0.45
ATOM	498	OD1	ASN 1 586	-11.610	20.195	-10.547	1.00	0.45
ATOM	499	ND2	ASN 1 586	-9.575	20.697	-9.668	1.00	0.45
ATOM	500	N	LEU 1 587	-9.231	16.473	-13.068	1.00	0.55
ATOM	501	CA	LEU 1 587	-8.562	15.751	-14.107	1.00	0.55
ATOM	502	C	LEU 1 587	-9.618	15.063	-14.928	1.00	0.55
ATOM	503	O	LEU 1 587	-10.739	14.850	-14.466	1.00	0.55
ATOM	504	CB	LEU 1 587	-7.668	14.679	-13.445	1.00	0.55
ATOM	505	CG	LEU 1 587	-6.461	14.146	-14.232	1.00	0.55
ATOM	506	CD1	LEU 1 587	-5.335	15.186	-14.287	1.00	0.55
ATOM	507	CD2	LEU 1 587	-5.960	12.826	-13.636	1.00	0.55
ATOM	508	N	HIS 1 588	-9.286	14.733	-16.194	1.00	0.46
ATOM	509	CA	HIS 1 588	-10.187	14.045	-17.076	1.00	0.46
ATOM	510	C	HIS 1 588	-10.210	12.614	-16.641	1.00	0.46
ATOM	511	O	HIS 1 588	-9.337	12.160	-15.904	1.00	0.46
ATOM	512	CB	HIS 1 588	-9.735	14.093	-18.548	1.00	0.46
ATOM	513	CG	HIS 1 588	-10.650	13.385	-19.503	1.00	0.46
ATOM	514	ND1	HIS 1 588	-10.514	12.066	-19.867	1.00	0.46
ATOM	515	CD2	HIS 1 588	-11.733	13.848	-20.188	1.00	0.46
ATOM	516	CE1	HIS 1 588	-11.511	11.795	-20.748	1.00	0.46
ATOM	517	NE2	HIS 1 588	-12.276	12.848	-20.974	1.00	0.46
ATOM	518	N	LEU 1 589	-11.222	11.856	-17.102	1.00	0.27
ATOM	519	CA	LEU 1 589	-11.395	10.496	-16.683	1.00	0.27
ATOM	520	C	LEU 1 589	-10.182	9.706	-17.062	1.00	0.27
ATOM	521	O	LEU 1 589	-9.646	8.945	-16.259	1.00	0.27
ATOM	522	CB	LEU 1 589	-12.588	9.823	-17.381	1.00	0.27
ATOM	523	CG	LEU 1 589	-12.792	8.365	-16.941	1.00	0.27
ATOM	524	CD1	LEU 1 589	-13.192	8.310	-15.463	1.00	0.27
ATOM	525	CD2	LEU 1 589	-13.781	7.624	-17.853	1.00	0.27
ATOM	526	N	ASP 1 590	-9.705	9.894	-18.303	1.00	0.25
ATOM	527	CA	ASP 1 590	-8.603	9.138	-18.816	1.00	0.25

150/208

ATOM	528	C	ASP	1	590	-7.387	9.404	-17.984	1.00	0.25
ATOM	529	O	ASP	1	590	-6.620	8.491	-17.685	1.00	0.25
ATOM	530	CB	ASP	1	590	-8.266	9.512	-20.271	1.00	0.25
ATOM	531	CG	ASP	1	590	-7.255	8.515	-20.817	1.00	0.25
ATOM	532	OD1	ASP	1	590	-6.868	7.583	-20.062	1.00	0.25
ATOM	533	OD2	ASP	1	590	-6.854	8.676	-22.000	1.00	0.25
ATOM	534	N	ASP	1	591	-7.173	10.673	-17.597	1.00	0.27
ATOM	535	CA	ASP	1	591	-6.010	11.033	-16.832	1.00	0.27
ATOM	536	C	ASP	1	591	-6.104	10.438	-15.472	1.00	0.27
ATOM	537	O	ASP	1	591	-5.102	10.074	-14.858	1.00	0.27
ATOM	538	CB	ASP	1	591	-5.840	12.551	-16.683	1.00	0.27
ATOM	539	CG	ASP	1	591	-5.433	13.097	-18.043	1.00	0.27
ATOM	540	OD1	ASP	1	591	-5.096	12.274	-18.935	1.00	0.27
ATOM	541	OD2	ASP	1	591	-5.449	14.346	-18.205	1.00	0.27
ATOM	542	N	GLN	1	592	-7.329	10.349	-14.945	1.00	0.31
ATOM	543	CA	GLN	1	592	-7.504	9.815	-13.638	1.00	0.31
ATOM	544	C	GLN	1	592	-7.058	8.389	-13.686	1.00	0.31
ATOM	545	O	GLN	1	592	-6.317	7.920	-12.824	1.00	0.31
ATOM	546	CB	GLN	1	592	-8.975	9.908	-13.238	1.00	0.31
ATOM	547	CG	GLN	1	592	-9.192	9.833	-11.742	1.00	0.31
ATOM	548	CD	GLN	1	592	-10.516	10.522	-11.463	1.00	0.31
ATOM	549	OE1	GLN	1	592	-11.571	9.893	-11.437	1.00	0.31
ATOM	550	NE2	GLN	1	592	-10.464	11.865	-11.264	1.00	0.31
ATOM	551	N	MET	1	593	-7.452	7.680	-14.758	1.00	0.38
ATOM	552	CA	MET	1	593	-7.117	6.295	-14.927	1.00	0.38
ATOM	553	C	MET	1	593	-5.622	6.167	-14.920	1.00	0.38
ATOM	554	O	MET	1	593	-5.081	5.268	-14.279	1.00	0.38
ATOM	555	CB	MET	1	593	-7.537	5.763	-16.303	1.00	0.38
ATOM	556	CG	MET	1	593	-9.038	5.737	-16.573	1.00	0.38
ATOM	557	SD	MET	1	593	-9.425	5.580	-18.341	1.00	0.38
ATOM	558	CE	MET	1	593	-8.466	4.055	-18.571	1.00	0.38
ATOM	559	N	THR	1	594	-4.908	7.070	-15.631	1.00	0.56
ATOM	560	CA	THR	1	594	-3.485	6.913	-15.743	1.00	0.56
ATOM	561	C	THR	1	594	-2.854	7.055	-14.395	1.00	0.56
ATOM	562	O	THR	1	594	-1.938	6.317	-14.040	1.00	0.56
ATOM	563	CB	THR	1	594	-2.822	7.881	-16.689	1.00	0.56
ATOM	564	OG1	THR	1	594	-1.494	7.455	-16.954	1.00	0.56
ATOM	565	CG2	THR	1	594	-2.784	9.284	-16.069	1.00	0.56
ATOM	566	N	LEU	1	595	-3.351	8.014	-13.606	1.00	0.67
ATOM	567	CA	LEU	1	595	-2.873	8.315	-12.298	1.00	0.67
ATOM	568	C	LEU	1	595	-3.015	7.054	-11.476	1.00	0.67
ATOM	569	O	LEU	1	595	-2.042	6.553	-10.914	1.00	0.67
ATOM	570	CB	LEU	1	595	-3.808	9.433	-11.781	1.00	0.67
ATOM	571	CG	LEU	1	595	-3.358	10.276	-10.593	1.00	0.67
ATOM	572	CD1	LEU	1	595	-3.379	9.462	-9.298	1.00	0.67
ATOM	573	CD2	LEU	1	595	-2.040	10.998	-10.916	1.00	0.67
ATOM	574	N	LEU	1	596	-4.221	6.451	-11.441	1.00	0.48
ATOM	575	CA	LEU	1	596	-4.421	5.274	-10.631	1.00	0.48
ATOM	576	C	LEU	1	596	-3.625	4.118	-11.126	1.00	0.48
ATOM	577	O	LEU	1	596	-3.050	3.384	-10.328	1.00	0.48
ATOM	578	CB	LEU	1	596	-5.871	4.749	-10.534	1.00	0.48
ATOM	579	CG	LEU	1	596	-6.844	5.622	-9.720	1.00	0.48
ATOM	580	CD1	LEU	1	596	-7.309	6.853	-10.504	1.00	0.48
ATOM	581	CD2	LEU	1	596	-8.006	4.788	-9.167	1.00	0.48
ATOM	582	N	GLN	1	597	-3.549	3.933	-12.453	1.00	0.43
ATOM	583	CA	GLN	1	597	-2.931	2.746	-12.967	1.00	0.43
ATOM	584	C	GLN	1	597	-1.514	2.677	-12.471	1.00	0.43
ATOM	585	O	GLN	1	597	-1.040	1.603	-12.105	1.00	0.43
ATOM	586	CB	GLN	1	597	-2.919	2.701	-14.499	1.00	0.43
ATOM	587	CG	GLN	1	597	-2.335	1.403	-15.054	1.00	0.43
ATOM	588	CD	GLN	1	597	-2.383	1.487	-16.570	1.00	0.43



151/208

ATOM	589	OE1 GLN 1 597	-2.999	2.391	-17.132	1.00	0.43
ATOM	590	NE2 GLN 1 597	-1.718	0.519	-17.255	1.00	0.43
ATOM	591	N TYR 1 598	-0.805	3.822	-12.449	1.00	0.63
ATOM	592	CA TYR 1 598	0.575	3.879	-12.039	1.00	0.63
ATOM	593	C TYR 1 598	0.754	3.705	-10.541	1.00	0.63
ATOM	594	O TYR 1 598	1.622	2.956	-10.095	1.00	0.63
ATOM	595	CB TYR 1 598	1.202	5.233	-12.413	1.00	0.63
ATOM	596	CG TYR 1 598	2.682	5.140	-12.280	1.00	0.63
ATOM	597	CD1 TYR 1 598	3.287	5.130	-11.044	1.00	0.63
ATOM	598	CD2 TYR 1 598	3.471	5.079	-13.406	1.00	0.63
ATOM	599	CE1 TYR 1 598	4.655	5.052	-10.936	1.00	0.63
ATOM	600	CE2 TYR 1 598	4.838	5.000	-13.304	1.00	0.63
ATOM	601	CZ TYR 1 598	5.433	4.983	-12.066	1.00	0.63
ATOM	602	OH TYR 1 598	6.837	4.903	-11.956	1.00	0.63
ATOM	603	N SER 1 599	-0.058	4.423	-9.734	1.00	0.57
ATOM	604	CA SER 1 599	0.007	4.569	-8.295	1.00	0.57
ATOM	605	C SER 1 599	-0.481	3.412	-7.472	1.00	0.57
ATOM	606	O SER 1 599	-0.041	3.263	-6.333	1.00	0.57
ATOM	607	CB SER 1 599	-0.841	5.750	-7.781	1.00	0.57
ATOM	608	OG SER 1 599	-0.367	6.985	-8.291	1.00	0.57
ATOM	609	N TRP 1 600	-1.382	2.566	-8.001	1.00	0.39
ATOM	610	CA TRP 1 600	-2.151	1.642	-7.200	1.00	0.39
ATOM	611	C TRP 1 600	-1.310	0.848	-6.233	1.00	0.39
ATOM	612	O TRP 1 600	-1.618	0.807	-5.043	1.00	0.39
ATOM	613	CB TRP 1 600	-2.900	0.632	-8.088	1.00	0.39
ATOM	614	CG TRP 1 600	-1.988	-0.338	-8.803	1.00	0.39
ATOM	615	CD1 TRP 1 600	-1.190	-0.146	-9.895	1.00	0.39
ATOM	616	CD2 TRP 1 600	-1.834	-1.714	-8.423	1.00	0.39
ATOM	617	NE1 TRP 1 600	-0.553	-1.321	-10.220	1.00	0.39
ATOM	618	CE2 TRP 1 600	-0.938	-2.293	-9.321	1.00	0.39
ATOM	619	CE3 TRP 1 600	-2.392	-2.436	-7.406	1.00	0.39
ATOM	620	CZ2 TRP 1 600	-0.589	-3.611	-9.217	1.00	0.39
ATOM	621	CZ3 TRP 1 600	-2.036	-3.763	-7.303	1.00	0.39
ATOM	622	CH2 TRP 1 600	-1.152	-4.338	-8.192	1.00	0.39
ATOM	623	N MET 1 601	-0.216	0.219	-6.690	1.00	0.53
ATOM	624	CA MET 1 601	0.564	-0.617	-5.819	1.00	0.53
ATOM	625	C MET 1 601	1.217	0.228	-4.766	1.00	0.53
ATOM	626	O MET 1 601	1.278	-0.154	-3.600	1.00	0.53
ATOM	627	CB MET 1 601	1.661	-1.370	-6.587	1.00	0.53
ATOM	628	CG MET 1 601	2.274	-2.606	-5.910	1.00	0.53
ATOM	629	SD MET 1 601	3.005	-2.371	-4.261	1.00	0.53
ATOM	630	CE MET 1 601	1.511	-2.869	-3.358	1.00	0.53
ATOM	631	N PHE 1 602	1.716	1.419	-5.147	1.00	0.69
ATOM	632	CA PHE 1 602	2.386	2.277	-4.208	1.00	0.69
ATOM	633	C PHE 1 602	1.406	2.538	-3.102	1.00	0.69
ATOM	634	O PHE 1 602	1.709	2.405	-1.917	1.00	0.69
ATOM	635	CB PHE 1 602	2.653	3.682	-4.783	1.00	0.69
ATOM	636	CG PHE 1 602	3.515	3.647	-5.996	1.00	0.69
ATOM	637	CD1 PHE 1 602	2.987	3.225	-7.192	1.00	0.69
ATOM	638	CD2 PHE 1 602	4.825	4.072	-5.957	1.00	0.69
ATOM	639	CE1 PHE 1 602	3.754	3.200	-8.331	1.00	0.69
ATOM	640	CE2 PHE 1 602	5.597	4.050	-7.096	1.00	0.69
ATOM	641	CZ PHE 1 602	5.062	3.615	-8.285	1.00	0.69
ATOM	642	N LEU 1 603	0.168	2.892	-3.473	1.00	0.63
ATOM	643	CA LEU 1 603	-0.807	3.239	-2.483	1.00	0.63
ATOM	644	C LEU 1 603	-1.101	2.078	-1.589	1.00	0.63
ATOM	645	O LEU 1 603	-1.198	2.243	-0.376	1.00	0.63
ATOM	646	CB LEU 1 603	-2.148	3.718	-3.063	1.00	0.63
ATOM	647	CG LEU 1 603	-2.117	5.146	-3.640	1.00	0.63
ATOM	648	CD1 LEU 1 603	-1.172	5.264	-4.843	1.00	0.63
ATOM	649	CD2 LEU 1 603	-3.536	5.648	-3.942	1.00	0.63

152/208

ATOM	650	N	MET 1 604	-1.252	0.867	-2.148	1.00	0.49
ATOM	651	CA	MET 1 604	-1.562	-0.244	-1.299	1.00	0.49
ATOM	652	C	MET 1 604	-0.425	-0.409	-0.343	1.00	0.49
ATOM	653	O	MET 1 604	-0.629	-0.699	0.835	1.00	0.49
ATOM	654	CB	MET 1 604	-1.713	-1.566	-2.070	1.00	0.49
ATOM	655	CG	MET 1 604	-2.928	-1.602	-2.999	1.00	0.49
ATOM	656	SD	MET 1 604	-3.371	-3.261	-3.593	1.00	0.49
ATOM	657	CE	MET 1 604	-4.703	-2.693	-4.687	1.00	0.49
ATOM	658	N	ALA 1 605	0.813	-0.234	-0.842	1.00	0.46
ATOM	659	CA	ALA 1 605	1.973	-0.428	-0.025	1.00	0.46
ATOM	660	C	ALA 1 605	2.080	0.598	1.060	1.00	0.46
ATOM	661	O	ALA 1 605	2.354	0.234	2.202	1.00	0.46
ATOM	662	CB	ALA 1 605	3.284	-0.438	-0.820	1.00	0.46
ATOM	663	N	PHE 1 606	1.856	1.899	0.761	1.00	0.53
ATOM	664	CA	PHE 1 606	1.972	2.853	1.833	1.00	0.53
ATOM	665	C	PHE 1 606	0.986	2.488	2.897	1.00	0.53
ATOM	666	O	PHE 1 606	1.304	2.529	4.080	1.00	0.53
ATOM	667	CB	PHE 1 606	1.665	4.323	1.489	1.00	0.53
ATOM	668	CG	PHE 1 606	2.879	4.986	0.949	1.00	0.53
ATOM	669	CD1	PHE 1 606	4.053	4.947	1.664	1.00	0.53
ATOM	670	CD2	PHE 1 606	2.835	5.709	-0.220	1.00	0.53
ATOM	671	CE1	PHE 1 606	5.185	5.570	1.198	1.00	0.53
ATOM	672	CE2	PHE 1 606	3.965	6.340	-0.684	1.00	0.53
ATOM	673	CZ	PHE 1 606	5.143	6.262	0.015	1.00	0.53
ATOM	674	N	ALA 1 607	-0.235	2.084	2.531	1.00	0.30
ATOM	675	CA	ALA 1 607	-1.186	1.776	3.560	1.00	0.30
ATOM	676	C	ALA 1 607	-0.664	0.648	4.398	1.00	0.30
ATOM	677	O	ALA 1 607	-0.782	0.671	5.624	1.00	0.30
ATOM	678	CB	ALA 1 607	-2.548	1.336	2.997	1.00	0.30
ATOM	679	N	LEU 1 608	-0.062	-0.373	3.759	1.00	0.08
ATOM	680	CA	LEU 1 608	0.419	-1.510	4.492	1.00	0.08
ATOM	681	C	LEU 1 608	1.488	-1.092	5.451	1.00	0.08
ATOM	682	O	LEU 1 608	1.457	-1.456	6.626	1.00	0.08
ATOM	683	CB	LEU 1 608	1.031	-2.598	3.589	1.00	0.08
ATOM	684	CG	LEU 1 608	1.572	-3.821	4.364	1.00	0.08
ATOM	685	CD1	LEU 1 608	0.457	-4.567	5.110	1.00	0.08
ATOM	686	CD2	LEU 1 608	2.388	-4.743	3.445	1.00	0.08
ATOM	687	N	GLY 1 609	2.461	-0.290	4.986	1.00	0.10
ATOM	688	CA	GLY 1 609	3.544	0.074	5.850	1.00	0.10
ATOM	689	C	GLY 1 609	3.006	0.831	7.024	1.00	0.10
ATOM	690	O	GLY 1 609	3.383	0.583	8.169	1.00	0.10
ATOM	691	N	TRP 1 610	2.087	1.776	6.766	1.00	0.19
ATOM	692	CA	TRP 1 610	1.563	2.603	7.814	1.00	0.19
ATOM	693	C	TRP 1 610	0.869	1.794	8.865	1.00	0.19
ATOM	694	O	TRP 1 610	1.122	1.963	10.058	1.00	0.19
ATOM	695	CB	TRP 1 610	0.576	3.658	7.279	1.00	0.19
ATOM	696	CG	TRP 1 610	-0.277	4.343	8.322	1.00	0.19
ATOM	697	CD1	TRP 1 610	-1.553	4.017	8.665	1.00	0.19
ATOM	698	CD2	TRP 1 610	0.088	5.465	9.148	1.00	0.19
ATOM	699	NE1	TRP 1 610	-2.010	4.864	9.645	1.00	0.19
ATOM	700	CE2	TRP 1 610	-1.011	5.758	9.955	1.00	0.19
ATOM	701	CE3	TRP 1 610	1.237	6.195	9.234	1.00	0.19
ATOM	702	CZ2	TRP 1 610	-0.976	6.783	10.855	1.00	0.19
ATOM	703	CZ3	TRP 1 610	1.272	7.227	10.145	1.00	0.19
ATOM	704	CH2	TRP 1 610	0.185	7.517	10.942	1.00	0.19
ATOM	705	N	ARG 1 611	-0.018	0.874	8.461	1.00	0.36
ATOM	706	CA	ARG 1 611	-0.765	0.113	9.420	1.00	0.36
ATOM	707	C	ARG 1 611	0.129	-0.825	10.166	1.00	0.36
ATOM	708	O	ARG 1 611	-0.172	-1.222	11.290	1.00	0.36
ATOM	709	CB	ARG 1 611	-1.947	-0.656	8.795	1.00	0.36
ATOM	710	CG	ARG 1 611	-1.594	-1.605	7.649	1.00	0.36

153/208

ATOM	711	CD	ARG	1	611	-2.843	-2.052	6.878	1.00	0.36
ATOM	712	NE	ARG	1	611	-2.414	-2.804	5.665	1.00	0.36
ATOM	713	CZ	ARG	1	611	-3.338	-3.131	4.715	1.00	0.36
ATOM	714	NH1	ARG	1	611	-4.631	-2.718	4.857	1.00	0.36
ATOM	715	NH2	ARG	1	611	-2.979	-3.868	3.623	1.00	0.36
ATOM	716	N	SER	1	612	1.225	-1.249	9.522	1.00	0.43
ATOM	717	CA	SER	1	612	2.174	-2.186	10.050	1.00	0.43
ATOM	718	C	SER	1	612	3.117	-1.602	11.065	1.00	0.43
ATOM	719	O	SER	1	612	3.787	-2.381	11.742	1.00	0.43
ATOM	720	CB	SER	1	612	2.991	-2.907	8.960	1.00	0.43
ATOM	721	OG	SER	1	612	3.707	-1.977	8.165	1.00	0.43
ATOM	722	N	TYR	1	613	3.223	-0.256	11.197	1.00	0.36
ATOM	723	CA	TYR	1	613	4.276	0.291	12.022	1.00	0.36
ATOM	724	C	TYR	1	613	4.237	-0.287	13.399	1.00	0.36
ATOM	725	O	TYR	1	613	5.247	-0.796	13.878	1.00	0.36
ATOM	726	CB	TYR	1	613	4.256	1.814	12.241	1.00	0.36
ATOM	727	CG	TYR	1	613	4.256	2.505	10.930	1.00	0.36
ATOM	728	CD1	TYR	1	613	5.079	2.095	9.908	1.00	0.36
ATOM	729	CD2	TYR	1	613	3.376	3.534	10.714	1.00	0.36
ATOM	730	CE1	TYR	1	613	5.053	2.732	8.690	1.00	0.36
ATOM	731	CE2	TYR	1	613	3.354	4.176	9.505	1.00	0.36
ATOM	732	CZ	TYR	1	613	4.189	3.781	8.489	1.00	0.36
ATOM	733	OH	TYR	1	613	4.146	4.451	7.248	1.00	0.36
ATOM	734	N	ARG	1	614	3.061	-0.308	14.042	1.00	0.35
ATOM	735	CA	ARG	1	614	3.003	-0.756	15.402	1.00	0.35
ATOM	736	C	ARG	1	614	3.435	-2.187	15.518	1.00	0.35
ATOM	737	O	ARG	1	614	4.107	-2.550	16.482	1.00	0.35
ATOM	738	CB	ARG	1	614	1.608	-0.581	16.027	1.00	0.35
ATOM	739	CG	ARG	1	614	1.273	0.899	16.238	1.00	0.35
ATOM	740	CD	ARG	1	614	0.000	1.165	17.044	1.00	0.35
ATOM	741	NE	ARG	1	614	-0.083	2.640	17.244	1.00	0.35
ATOM	742	CZ	ARG	1	614	-1.118	3.186	17.948	1.00	0.35
ATOM	743	NH1	ARG	1	614	-2.094	2.383	18.461	1.00	0.35
ATOM	744	NH2	ARG	1	614	-1.175	4.536	18.139	1.00	0.35
ATOM	745	N	GLN	1	615	3.075	-3.054	14.552	1.00	0.40
ATOM	746	CA	GLN	1	615	3.466	-4.428	14.697	1.00	0.40
ATOM	747	C	GLN	1	615	4.811	-4.597	14.072	1.00	0.40
ATOM	748	O	GLN	1	615	4.927	-4.855	12.876	1.00	0.40
ATOM	749	CB	GLN	1	615	2.505	-5.418	14.012	1.00	0.40
ATOM	750	CG	GLN	1	615	1.105	-5.450	14.637	1.00	0.40
ATOM	751	CD	GLN	1	615	0.327	-4.230	14.160	1.00	0.40
ATOM	752	OE1	GLN	1	615	-0.699	-3.875	14.736	1.00	0.40
ATOM	753	NE2	GLN	1	615	0.820	-3.575	13.076	1.00	0.40
ATOM	754	N	SER	1	616	5.871	-4.490	14.893	1.00	0.38
ATOM	755	CA	SER	1	616	7.205	-4.567	14.381	1.00	0.38
ATOM	756	C	SER	1	616	7.603	-5.993	14.244	1.00	0.38
ATOM	757	O	SER	1	616	7.004	-6.872	14.861	1.00	0.38
ATOM	758	CB	SER	1	616	8.246	-3.885	15.283	1.00	0.38
ATOM	759	OG	SER	1	616	8.331	-4.563	16.528	1.00	0.38
ATOM	760	N	SER	1	617	8.618	-6.216	13.380	1.00	0.34
ATOM	761	CA	SER	1	617	9.277	-7.462	13.112	1.00	0.34
ATOM	762	C	SER	1	617	9.101	-7.783	11.679	1.00	0.34
ATOM	763	O	SER	1	617	8.136	-7.370	11.044	1.00	0.34
ATOM	764	CB	SER	1	617	8.794	-8.691	13.909	1.00	0.34
ATOM	765	OG	SER	1	617	9.025	-8.493	15.296	1.00	0.34
ATOM	766	N	ALA	1	618	10.038	-8.574	11.133	1.00	0.31
ATOM	767	CA	ALA	1	618	9.912	-8.986	9.772	1.00	0.31
ATOM	768	C	ALA	1	618	8.631	-9.736	9.743	1.00	0.31
ATOM	769	O	ALA	1	618	7.901	-9.753	8.753	1.00	0.31
ATOM	770	CB	ALA	1	618	11.029	-9.947	9.330	1.00	0.31
ATOM	771	N	ASN	1	619	8.349	-10.365	10.891	1.00	0.35

SUBSTITUTE SHEET (RULE 26)

154/208

ATOM	772	CA	ASN 1 619	7.190	-11.142	11.140	1.00	0.35
ATOM	773	C	ASN 1 619	5.960	-10.277	11.190	1.00	0.35
ATOM	774	O	ASN 1 619	4.845	-10.793	11.173	1.00	0.35
ATOM	775	CB	ASN 1 619	7.280	-11.924	12.461	1.00	0.35
ATOM	776	CG	ASN 1 619	8.427	-12.924	12.335	1.00	0.35
ATOM	777	OD1	ASN 1 619	9.382	-12.881	13.109	1.00	0.35
ATOM	778	ND2	ASN 1 619	8.339	-13.845	11.338	1.00	0.35
ATOM	779	N	LEU 1 620	6.076	-8.940	11.292	1.00	0.39
ATOM	780	CA	LEU 1 620	4.804	-8.298	11.401	1.00	0.39
ATOM	781	C	LEU 1 620	4.526	-7.328	10.294	1.00	0.39
ATOM	782	O	LEU 1 620	5.102	-6.243	10.228	1.00	0.39
ATOM	783	CB	LEU 1 620	4.612	-7.574	12.743	1.00	0.39
ATOM	784	CG	LEU 1 620	4.585	-8.531	13.951	1.00	0.39
ATOM	785	CD1	LEU 1 620	3.372	-9.470	13.893	1.00	0.39
ATOM	786	CD2	LEU 1 620	5.911	-9.294	14.094	1.00	0.39
ATOM	787	N	LEU 1 621	3.606	-7.728	9.391	1.00	0.36
ATOM	788	CA	LEU 1 621	3.051	-6.876	8.378	1.00	0.36
ATOM	789	C	LEU 1 621	1.576	-7.096	8.477	1.00	0.36
ATOM	790	O	LEU 1 621	1.109	-8.233	8.431	1.00	0.36
ATOM	791	CB	LEU 1 621	3.454	-7.225	6.936	1.00	0.36
ATOM	792	CG	LEU 1 621	4.927	-6.933	6.605	1.00	0.36
ATOM	793	CD1	LEU 1 621	5.248	-7.307	5.150	1.00	0.36
ATOM	794	CD2	LEU 1 621	5.296	-5.479	6.940	1.00	0.36
ATOM	795	N	CYS 1 622	0.790	-6.014	8.626	1.00	0.33
ATOM	796	CA	CYS 1 622	-0.619	-6.208	8.778	1.00	0.33
ATOM	797	C	CYS 1 622	-1.297	-6.000	7.469	1.00	0.33
ATOM	798	O	CYS 1 622	-1.742	-4.897	7.161	1.00	0.33
ATOM	799	CB	CYS 1 622	-1.277	-5.221	9.753	1.00	0.33
ATOM	800	SG	CYS 1 622	-0.819	-5.533	11.478	1.00	0.33
ATOM	801	N	PHE 1 623	-1.427	-7.066	6.663	1.00	0.23
ATOM	802	CA	PHE 1 623	-2.157	-6.892	5.446	1.00	0.23
ATOM	803	C	PHE 1 623	-3.554	-6.558	5.847	1.00	0.23
ATOM	804	O	PHE 1 623	-4.206	-5.711	5.237	1.00	0.23
ATOM	805	CB	PHE 1 623	-2.223	-8.146	4.554	1.00	0.23
ATOM	806	CG	PHE 1 623	-0.889	-8.312	3.914	1.00	0.23
ATOM	807	CD1	PHE 1 623	-0.599	-7.645	2.748	1.00	0.23
ATOM	808	CD2	PHE 1 623	0.077	-9.109	4.477	1.00	0.23
ATOM	809	CE1	PHE 1 623	0.627	-7.783	2.141	1.00	0.23
ATOM	810	CE2	PHE 1 623	1.304	-9.251	3.874	1.00	0.23
ATOM	811	CZ	PHE 1 623	1.586	-8.588	2.704	1.00	0.23
ATOM	812	N	ALA 1 624	-4.046	-7.248	6.892	1.00	0.28
ATOM	813	CA	ALA 1 624	-5.351	-7.021	7.439	1.00	0.28
ATOM	814	C	ALA 1 624	-5.229	-7.359	8.890	1.00	0.28
ATOM	815	O	ALA 1 624	-4.285	-8.041	9.285	1.00	0.28
ATOM	816	CB	ALA 1 624	-6.438	-7.938	6.848	1.00	0.28
ATOM	817	N	PRO 1 625	-6.130	-6.898	9.714	1.00	0.58
ATOM	818	CA	PRO 1 625	-6.054	-7.227	11.107	1.00	0.58
ATOM	819	C	PRO 1 625	-6.288	-8.688	11.219	1.00	0.58
ATOM	820	O	PRO 1 625	-5.817	-9.328	12.159	1.00	0.58
ATOM	821	CB	PRO 1 625	-7.083	-6.329	11.806	1.00	0.58
ATOM	822	CG	PRO 1 625	-7.869	-5.658	10.659	1.00	0.58
ATOM	823	CD	PRO 1 625	-6.896	-5.691	9.471	1.00	0.58
ATOM	824	N	ASP 1 626	-7.035	-9.206	10.241	1.00	0.59
ATOM	825	CA	ASP 1 626	-7.416	-10.568	10.093	1.00	0.59
ATOM	826	C	ASP 1 626	-6.220	-11.387	9.713	1.00	0.59
ATOM	827	O	ASP 1 626	-6.154	-12.571	10.037	1.00	0.59
ATOM	828	CB	ASP 1 626	-8.458	-10.697	8.972	1.00	0.59
ATOM	829	CG	ASP 1 626	-9.119	-12.035	9.151	1.00	0.59
ATOM	830	OD1	ASP 1 626	-8.700	-12.723	10.116	1.00	0.59
ATOM	831	OD2	ASP 1 626	-10.033	-12.389	8.359	1.00	0.59
ATOM	832	N	LEU 1 627	-5.262	-10.799	8.959	1.00	0.40

155/208

ATOM	833	CA	LEU 1 627	-4.156	-11.601	8.517	1.00	0.40
ATOM	834	C	LEU 1 627	-2.873	-10.863	8.760	1.00	0.40
ATOM	835	O	LEU 1 627	-2.474	-10.015	7.967	1.00	0.40
ATOM	836	CB	LEU 1 627	-4.237	-11.897	7.006	1.00	0.40
ATOM	837	CG	LEU 1 627	-3.086	-12.752	6.449	1.00	0.40
ATOM	838	CD1	LEU 1 627	-3.121	-14.176	7.031	1.00	0.40
ATOM	839	CD2	LEU 1 627	-3.074	-12.736	4.911	1.00	0.40
ATOM	840	N	ILE 1 628	-2.165	-11.203	9.856	1.00	0.54
ATOM	841	CA	ILE 1 628	-0.900	-10.585	10.128	1.00	0.54
ATOM	842	C	ILE 1 628	0.130	-11.549	9.617	1.00	0.54
ATOM	843	O	ILE 1 628	0.138	-12.727	9.968	1.00	0.54
ATOM	844	CB	ILE 1 628	-0.685	-10.303	11.591	1.00	0.54
ATOM	845	CG1	ILE 1 628	0.537	-9.397	11.795	1.00	0.54
ATOM	846	CG2	ILE 1 628	-0.632	-11.634	12.360	1.00	0.54
ATOM	847	CD1	ILE 1 628	0.594	-8.779	13.191	1.00	0.54
ATOM	848	N	ILE 1 629	1.027	-11.047	8.752	1.00	0.64
ATOM	849	CA	ILE 1 629	1.979	-11.834	8.023	1.00	0.64
ATOM	850	C	ILE 1 629	3.342	-11.573	8.573	1.00	0.64
ATOM	851	O	ILE 1 629	3.671	-10.449	8.948	1.00	0.64
ATOM	852	CB	ILE 1 629	1.927	-11.403	6.579	1.00	0.64
ATOM	853	CG1	ILE 1 629	2.792	-12.233	5.626	1.00	0.64
ATOM	854	CG2	ILE 1 629	2.287	-9.911	6.572	1.00	0.64
ATOM	855	CD1	ILE 1 629	4.281	-11.955	5.781	1.00	0.64
ATOM	856	N	ASN 1 630	4.169	-12.635	8.633	1.00	0.41
ATOM	857	CA	ASN 1 630	5.482	-12.552	9.194	1.00	0.41
ATOM	858	C	ASN 1 630	6.475	-12.894	8.133	1.00	0.41
ATOM	859	O	ASN 1 630	6.129	-13.466	7.103	1.00	0.41
ATOM	860	CB	ASN 1 630	5.654	-13.509	10.396	1.00	0.41
ATOM	861	CG	ASN 1 630	5.480	-14.950	9.969	1.00	0.41
ATOM	862	OD1	ASN 1 630	5.193	-15.240	8.812	1.00	0.41
ATOM	863	ND2	ASN 1 630	5.644	-15.888	10.938	1.00	0.41
ATOM	864	N	GLU 1 631	7.758	-12.570	8.376	1.00	0.35
ATOM	865	CA	GLU 1 631	8.759	-12.772	7.371	1.00	0.35
ATOM	866	C	GLU 1 631	8.763	-14.218	6.985	1.00	0.35
ATOM	867	O	GLU 1 631	8.946	-14.556	5.819	1.00	0.35
ATOM	868	CB	GLU 1 631	10.186	-12.437	7.834	1.00	0.35
ATOM	869	CG	GLU 1 631	10.707	-13.352	8.945	1.00	0.35
ATOM	870	CD	GLU 1 631	12.203	-13.111	9.077	1.00	0.35
ATOM	871	OE1	GLU 1 631	12.733	-12.257	8.317	1.00	0.35
ATOM	872	OE2	GLU 1 631	12.839	-13.780	9.934	1.00	0.35
ATOM	873	N	GLN 1 632	8.557	-15.133	7.941	1.00	0.52
ATOM	874	CA	GLN 1 632	8.618	-16.517	7.571	1.00	0.52
ATOM	875	C	GLN 1 632	7.574	-16.821	6.535	1.00	0.52
ATOM	876	O	GLN 1 632	7.866	-17.470	5.531	1.00	0.52
ATOM	877	CB	GLN 1 632	8.368	-17.464	8.756	1.00	0.52
ATOM	878	CG	GLN 1 632	9.510	-17.490	9.774	1.00	0.52
ATOM	879	CD	GLN 1 632	10.662	-18.261	9.145	1.00	0.52
ATOM	880	OE1	GLN 1 632	11.721	-18.428	9.747	1.00	0.52
ATOM	881	NE2	GLN 1 632	10.448	-18.754	7.895	1.00	0.52
ATOM	882	N	ARG 1 633	6.333	-16.344	6.737	1.00	0.65
ATOM	883	CA	ARG 1 633	5.256	-16.668	5.845	1.00	0.65
ATOM	884	C	ARG 1 633	5.429	-16.003	4.512	1.00	0.65
ATOM	885	O	ARG 1 633	4.965	-16.513	3.496	1.00	0.65
ATOM	886	CB	ARG 1 633	3.849	-16.355	6.388	1.00	0.65
ATOM	887	CG	ARG 1 633	3.556	-14.883	6.649	1.00	0.65
ATOM	888	CD	ARG 1 633	2.143	-14.652	7.187	1.00	0.65
ATOM	889	NE	ARG 1 633	2.200	-14.773	8.672	1.00	0.65
ATOM	890	CZ	ARG 1 633	2.009	-15.985	9.271	1.00	0.65
ATOM	891	NH1	ARG 1 633	1.776	-17.093	8.509	1.00	0.65
ATOM	892	NH2	ARG 1 633	2.050	-16.087	10.631	1.00	0.65
ATOM	893	N	MET 1 634	6.112	-14.849	4.465	1.00	0.68

SUBSTITUTE SHEET (RULE 26)

156/208

ATOM	894	CA	MET	1	634	6.269	-14.113	3.239	1.00	0.68
ATOM	895	C	MET	1	634	6.987	-14.978	2.246	1.00	0.68
ATOM	896	O	MET	1	634	6.900	-14.757	1.039	1.00	0.68
ATOM	897	CB	MET	1	634	7.101	-12.828	3.408	1.00	0.68
ATOM	898	CG	MET	1	634	8.600	-13.100	3.547	1.00	0.68
ATOM	899	SD	MET	1	634	9.560	-11.763	4.321	1.00	0.68
ATOM	900	CE	MET	1	634	10.886	-12.819	4.967	1.00	0.68
ATOM	901	N	THR	1	635	7.711	-15.993	2.745	1.00	0.73
ATOM	902	CA	THR	1	635	8.559	-16.864	1.977	1.00	0.73
ATOM	903	C	THR	1	635	7.806	-17.553	0.873	1.00	0.73
ATOM	904	O	THR	1	635	8.424	-17.994	-0.094	1.00	0.73
ATOM	905	CB	THR	1	635	9.194	-17.939	2.807	1.00	0.73
ATOM	906	OG1	THR	1	635	10.204	-18.603	2.060	1.00	0.73
ATOM	907	CG2	THR	1	635	8.106	-18.942	3.230	1.00	0.73
ATOM	908	N	LEU	1	636	6.469	-17.684	0.969	1.00	0.86
ATOM	909	CA	LEU	1	636	5.751	-18.430	-0.032	1.00	0.86
ATOM	910	C	LEU	1	636	6.039	-17.924	-1.433	1.00	0.86
ATOM	911	O	LEU	1	636	6.092	-18.772	-2.322	1.00	0.86
ATOM	912	CB	LEU	1	636	4.229	-18.455	0.191	1.00	0.86
ATOM	913	CG	LEU	1	636	3.802	-19.425	1.312	1.00	0.86
ATOM	914	CD1	LEU	1	636	4.438	-19.066	2.661	1.00	0.86
ATOM	915	CD2	LEU	1	636	2.275	-19.537	1.396	1.00	0.86
ATOM	916	N	PRO	1	637	6.111	-16.634	-1.719	1.00	0.89
ATOM	917	CA	PRO	1	637	6.582	-16.193	-3.029	1.00	0.89
ATOM	918	C	PRO	1	637	7.954	-15.629	-2.840	1.00	0.89
ATOM	919	O	PRO	1	637	8.410	-15.566	-1.705	1.00	0.89
ATOM	920	CB	PRO	1	637	5.629	-15.087	-3.481	1.00	0.89
ATOM	921	CG	PRO	1	637	4.391	-15.244	-2.588	1.00	0.89
ATOM	922	CD	PRO	1	637	4.954	-15.859	-1.299	1.00	0.89
ATOM	923	N	CYS	1	638	8.632	-15.137	-3.899	1.00	0.83
ATOM	924	CA	CYS	1	638	9.892	-14.475	-3.665	1.00	0.83
ATOM	925	C	CYS	1	638	9.581	-13.084	-3.175	1.00	0.83
ATOM	926	O	CYS	1	638	10.144	-12.095	-3.645	1.00	0.83
ATOM	927	CB	CYS	1	638	10.749	-14.344	-4.937	1.00	0.83
ATOM	928	SG	CYS	1	638	9.943	-13.342	-6.223	1.00	0.83
ATOM	929	N	MET	1	639	8.647	-13.005	-2.208	1.00	0.83
ATOM	930	CA	MET	1	639	8.116	-11.864	-1.524	1.00	0.83
ATOM	931	C	MET	1	639	9.159	-11.384	-0.570	1.00	0.83
ATOM	932	O	MET	1	639	9.200	-10.210	-0.221	1.00	0.83
ATOM	933	CB	MET	1	639	6.911	-12.243	-0.642	1.00	0.83
ATOM	934	CG	MET	1	639	5.951	-11.093	-0.332	1.00	0.83
ATOM	935	SD	MET	1	639	4.622	-10.856	-1.556	1.00	0.83
ATOM	936	CE	MET	1	639	5.572	-11.366	-3.016	1.00	0.83
ATOM	937	N	TYR	1	640	10.041	-12.301	-0.142	1.00	0.81
ATOM	938	CA	TYR	1	640	10.993	-12.101	0.914	1.00	0.81
ATOM	939	C	TYR	1	640	11.701	-10.796	0.742	1.00	0.81
ATOM	940	O	TYR	1	640	11.752	-9.991	1.673	1.00	0.81
ATOM	941	CB	TYR	1	640	12.046	-13.227	0.874	1.00	0.81
ATOM	942	CG	TYR	1	640	13.176	-12.967	1.810	1.00	0.81
ATOM	943	CD1	TYR	1	640	13.113	-13.365	3.122	1.00	0.81
ATOM	944	CD2	TYR	1	640	14.316	-12.340	1.361	1.00	0.81
ATOM	945	CE1	TYR	1	640	14.160	-13.132	3.982	1.00	0.81
ATOM	946	CE2	TYR	1	640	15.367	-12.103	2.213	1.00	0.81
ATOM	947	CZ	TYR	1	640	15.290	-12.500	3.526	1.00	0.81
ATOM	948	OH	TYR	1	640	16.369	-12.260	4.403	1.00	0.81
ATOM	949	N	ASP	1	641	12.237	-10.525	-0.455	1.00	0.63
ATOM	950	CA	ASP	1	641	12.986	-9.314	-0.604	1.00	0.63
ATOM	951	C	ASP	1	641	12.114	-8.124	-0.342	1.00	0.63
ATOM	952	O	ASP	1	641	12.479	-7.252	0.444	1.00	0.63
ATOM	953	CB	ASP	1	641	13.614	-9.163	-2.002	1.00	0.63
ATOM	954	CG	ASP	1	641	12.512	-9.127	-3.054	1.00	0.63

157/208

ATOM	955	OD1 ASP 1 641	11.468	-9.804	-2.855	1.00	0.63
ATOM	956	OD2 ASP 1 641	12.702	-8.415	-4.077	1.00	0.63
ATOM	957	N GLN 1 642	10.927	-8.061	-0.971	1.00	0.38
ATOM	958	CA GLN 1 642	10.081	-6.911	-0.818	1.00	0.38
ATOM	959	C GLN 1 642	9.535	-6.842	0.573	1.00	0.38
ATOM	960	O GLN 1 642	9.455	-5.769	1.166	1.00	0.38
ATOM	961	CB GLN 1 642	8.901	-6.886	-1.805	1.00	0.38
ATOM	962	CG GLN 1 642	7.900	-8.030	-1.641	1.00	0.38
ATOM	963	CD GLN 1 642	6.823	-7.829	-2.700	1.00	0.38
ATOM	964	OE1 GLN 1 642	5.800	-8.511	-2.711	1.00	0.38
ATOM	965	NE2 GLN 1 642	7.061	-6.858	-3.622	1.00	0.38
ATOM	966	N CYS 1 643	9.164	-7.995	1.145	1.00	0.24
ATOM	967	CA CYS 1 643	8.557	-7.993	2.439	1.00	0.24
ATOM	968	C CYS 1 643	9.519	-7.380	3.393	1.00	0.24
ATOM	969	O CYS 1 643	9.125	-6.579	4.239	1.00	0.24
ATOM	970	CB CYS 1 643	8.202	-9.401	2.928	1.00	0.24
ATOM	971	SG CYS 1 643	7.433	-9.392	4.575	1.00	0.24
ATOM	972	N LYS 1 644	10.814	-7.727	3.277	1.00	0.26
ATOM	973	CA LYS 1 644	11.765	-7.146	4.177	1.00	0.26
ATOM	974	C LYS 1 644	11.804	-5.669	3.942	1.00	0.26
ATOM	975	O LYS 1 644	11.795	-4.888	4.892	1.00	0.26
ATOM	976	CB LYS 1 644	13.197	-7.679	4.004	1.00	0.26
ATOM	977	CG LYS 1 644	13.377	-9.124	4.470	1.00	0.26
ATOM	978	CD LYS 1 644	14.778	-9.673	4.194	1.00	0.26
ATOM	979	CE LYS 1 644	15.843	-9.093	5.128	1.00	0.26
ATOM	980	NZ LYS 1 644	17.170	-9.665	4.809	1.00	0.26
ATOM	981	N HIS 1 645	11.820	-5.237	2.665	1.00	0.33
ATOM	982	CA HIS 1 645	11.905	-3.827	2.417	1.00	0.33
ATOM	983	C HIS 1 645	10.707	-3.166	3.024	1.00	0.33
ATOM	984	O HIS 1 645	10.823	-2.137	3.686	1.00	0.33
ATOM	985	CB HIS 1 645	11.985	-3.468	0.924	1.00	0.33
ATOM	986	CG HIS 1 645	13.330	-3.796	0.341	1.00	0.33
ATOM	987	ND1 HIS 1 645	13.639	-4.977	-0.296	1.00	0.33
ATOM	988	CD2 HIS 1 645	14.477	-3.062	0.333	1.00	0.33
ATOM	989	CE1 HIS 1 645	14.945	-4.899	-0.655	1.00	0.33
ATOM	990	NE2 HIS 1 645	15.497	-3.754	-0.293	1.00	0.33
ATOM	991	N MET 1 646	9.522	-3.770	2.850	1.00	0.28
ATOM	992	CA MET 1 646	8.324	-3.212	3.401	1.00	0.28
ATOM	993	C MET 1 646	8.498	-3.168	4.887	1.00	0.28
ATOM	994	O MET 1 646	8.093	-2.216	5.553	1.00	0.28
ATOM	995	CB MET 1 646	7.085	-4.072	3.102	1.00	0.28
ATOM	996	CG MET 1 646	6.769	-4.179	1.609	1.00	0.28
ATOM	997	SD MET 1 646	5.313	-5.191	1.211	1.00	0.28
ATOM	998	CE MET 1 646	5.515	-5.055	-0.588	1.00	0.28
ATOM	999	N LEU 1 647	9.135	-4.203	5.453	1.00	0.37
ATOM	1000	CA LEU 1 647	9.302	-4.259	6.877	1.00	0.37
ATOM	1001	C LEU 1 647	10.067	-3.044	7.293	1.00	0.37
ATOM	1002	O LEU 1 647	9.695	-2.348	8.239	1.00	0.37
ATOM	1003	CB LEU 1 647	10.155	-5.470	7.283	1.00	0.37
ATOM	1004	CG LEU 1 647	9.510	-6.823	6.937	1.00	0.37
ATOM	1005	CD1 LEU 1 647	10.517	-7.972	7.083	1.00	0.37
ATOM	1006	CD2 LEU 1 647	8.221	-7.048	7.744	1.00	0.37
ATOM	1007	N TYR 1 648	11.150	-2.750	6.552	1.00	0.59
ATOM	1008	CA TYR 1 648	12.029	-1.671	6.883	1.00	0.59
ATOM	1009	C TYR 1 648	11.295	-0.372	6.764	1.00	0.59
ATOM	1010	O TYR 1 648	11.471	0.520	7.593	1.00	0.59
ATOM	1011	CB TYR 1 648	13.257	-1.613	5.958	1.00	0.59
ATOM	1012	CG TYR 1 648	14.105	-0.469	6.394	1.00	0.59
ATOM	1013	CD1 TYR 1 648	13.869	0.806	5.932	1.00	0.59
ATOM	1014	CD2 TYR 1 648	15.140	-0.677	7.274	1.00	0.59
ATOM	1015	CE1 TYR 1 648	14.656	1.855	6.342	1.00	0.59

158/208

ATOM	1016	CE2 TYR 1 648	15.932	0.368	7.689	1.00	0.59
ATOM	1017	CZ TYR 1 648	15.689	1.636	7.222	1.00	0.59
ATOM	1018	OH TYR 1 648	16.499	2.713	7.644	1.00	0.59
ATOM	1019	N VAL 1 649	10.440	-0.215	5.737	1.00	0.47
ATOM	1020	CA VAL 1 649	9.815	1.070	5.594	1.00	0.47
ATOM	1021	C VAL 1 649	8.989	1.394	6.805	1.00	0.47
ATOM	1022	O VAL 1 649	9.124	2.473	7.373	1.00	0.47
ATOM	1023	CB VAL 1 649	8.949	1.194	4.368	1.00	0.47
ATOM	1024	CG1 VAL 1 649	7.719	0.283	4.498	1.00	0.47
ATOM	1025	CG2 VAL 1 649	8.591	2.680	4.187	1.00	0.47
ATOM	1026	N SER 1 650	8.143	0.468	7.285	1.00	0.27
ATOM	1027	CA SER 1 650	7.306	0.811	8.402	1.00	0.27
ATOM	1028	C SER 1 650	8.180	1.111	9.573	1.00	0.27
ATOM	1029	O SER 1 650	7.870	1.984	10.385	1.00	0.27
ATOM	1030	CB SER 1 650	6.341	-0.324	8.797	1.00	0.27
ATOM	1031	OG SER 1 650	7.061	-1.448	9.279	1.00	0.27
ATOM	1032	N SER 1 651	9.308	0.391	9.701	1.00	0.27
ATOM	1033	CA SER 1 651	10.133	0.627	10.846	1.00	0.27
ATOM	1034	C SER 1 651	10.635	2.032	10.785	1.00	0.27
ATOM	1035	O SER 1 651	10.673	2.728	11.799	1.00	0.27
ATOM	1036	CB SER 1 651	11.336	-0.332	10.964	1.00	0.27
ATOM	1037	OG SER 1 651	12.300	-0.081	9.954	1.00	0.27
ATOM	1038	N GLU 1 652	11.015	2.499	9.582	1.00	0.28
ATOM	1039	CA GLU 1 652	11.531	3.830	9.462	1.00	0.28
ATOM	1040	C GLU 1 652	10.443	4.785	9.825	1.00	0.28
ATOM	1041	O GLU 1 652	10.691	5.801	10.469	1.00	0.28
ATOM	1042	CB GLU 1 652	12.038	4.159	8.047	1.00	0.28
ATOM	1043	CG GLU 1 652	12.859	5.451	7.989	1.00	0.28
ATOM	1044	CD GLU 1 652	13.572	5.497	6.646	1.00	0.28
ATOM	1045	OE1 GLU 1 652	13.370	4.553	5.836	1.00	0.28
ATOM	1046	OE2 GLU 1 652	14.332	6.475	6.413	1.00	0.28
ATOM	1047	N LEU 1 653	9.192	4.485	9.431	1.00	0.34
ATOM	1048	CA LEU 1 653	8.137	5.394	9.768	1.00	0.34
ATOM	1049	C LEU 1 653	7.999	5.464	11.253	1.00	0.34
ATOM	1050	O LEU 1 653	7.721	6.536	11.790	1.00	0.34
ATOM	1051	CB LEU 1 653	6.785	5.063	9.134	1.00	0.34
ATOM	1052	CG LEU 1 653	6.705	5.465	7.648	1.00	0.34
ATOM	1053	CD1 LEU 1 653	6.707	6.993	7.496	1.00	0.34
ATOM	1054	CD2 LEU 1 653	7.799	4.799	6.804	1.00	0.34
ATOM	1055	N HIS 1 654	8.171	4.335	11.973	1.00	0.45
ATOM	1056	CA HIS 1 654	8.119	4.466	13.401	1.00	0.45
ATOM	1057	C HIS 1 654	9.228	5.343	13.852	1.00	0.45
ATOM	1058	O HIS 1 654	9.014	6.248	14.656	1.00	0.45
ATOM	1059	CB HIS 1 654	8.345	3.192	14.220	1.00	0.45
ATOM	1060	CG HIS 1 654	7.108	2.675	14.865	1.00	0.45
ATOM	1061	ND1 HIS 1 654	6.329	3.395	15.744	1.00	0.45
ATOM	1062	CD2 HIS 1 654	6.539	1.451	14.785	1.00	0.45
ATOM	1063	CE1 HIS 1 654	5.330	2.571	16.148	1.00	0.45
ATOM	1064	NE2 HIS 1 654	5.416	1.377	15.590	1.00	0.45
ATOM	1065	N ARG 1 655	10.440	5.109	13.317	1.00	0.58
ATOM	1066	CA ARG 1 655	11.582	5.841	13.780	1.00	0.58
ATOM	1067	C ARG 1 655	11.304	7.297	13.588	1.00	0.58
ATOM	1068	O ARG 1 655	11.511	8.106	14.489	1.00	0.58
ATOM	1069	CB ARG 1 655	12.862	5.497	13.001	1.00	0.58
ATOM	1070	CG ARG 1 655	13.315	4.046	13.187	1.00	0.58
ATOM	1071	CD ARG 1 655	14.588	3.696	12.415	1.00	0.58
ATOM	1072	NE ARG 1 655	15.730	4.359	13.105	1.00	0.58
ATOM	1073	CZ ARG 1 655	16.357	3.731	14.141	1.00	0.58
ATOM	1074	NH1 ARG 1 655	15.945	2.493	14.540	1.00	0.58
ATOM	1075	NH2 ARG 1 655	17.400	4.340	14.778	1.00	0.58
ATOM	1076	N LEU 1 656	10.783	7.659	12.406	1.00	0.65



15A/208

ATOM 1077 CA LEU 1 656	10.457	9.023	12.107	1.00	0.65
ATOM 1078 C LEU 1 656	9.298	9.465	12.943	1.00	0.65
ATOM 1079 O LEU 1 656	9.103	10.663	13.143	1.00	0.65
ATOM 1080 CB LEU 1 656	10.115	9.278	10.627	1.00	0.65
ATOM 1081 CG LEU 1 656	11.347	9.325	9.698	1.00	0.65
ATOM 1082 CD1 LEU 1 656	12.123	8.001	9.689	1.00	0.65
ATOM 1083 CD2 LEU 1 656	10.954	9.789	8.287	1.00	0.65
ATOM 1084 N GLN 1 657	8.485	8.516	13.445	1.00	0.65
ATOM 1085 CA GLN 1 657	7.319	8.910	14.179	1.00	0.65
ATOM 1086 C GLN 1 657	6.418	9.589	13.207	1.00	0.65
ATOM 1087 O GLN 1 657	5.896	10.673	13.462	1.00	0.65
ATOM 1088 CB GLN 1 657	7.620	9.893	15.324	1.00	0.65
ATOM 1089 CG GLN 1 657	8.497	9.301	16.429	1.00	0.65
ATOM 1090 CD GLN 1 657	8.712	10.375	17.486	1.00	0.65
ATOM 1091 OE1 GLN 1 657	9.386	10.151	18.490	1.00	0.65
ATOM 1092 NE2 GLN 1 657	8.124	11.582	17.257	1.00	0.65
ATOM 1093 N VAL 1 658	6.212	8.936	12.049	1.00	0.48
ATOM 1094 CA VAL 1 658	5.390	9.515	11.028	1.00	0.48
ATOM 1095 C VAL 1 658	4.052	9.814	11.615	1.00	0.48
ATOM 1096 O VAL 1 658	3.559	9.094	12.481	1.00	0.48
ATOM 1097 CB VAL 1 658	5.186	8.627	9.835	1.00	0.48
ATOM 1098 CG1 VAL 1 658	4.409	7.379	10.285	1.00	0.48
ATOM 1099 CG2 VAL 1 658	4.476	9.439	8.740	1.00	0.48
ATOM 1100 N SER 1 659	3.433	10.913	11.145	1.00	0.33
ATOM 1101 CA SER 1 659	2.174	11.328	11.685	1.00	0.33
ATOM 1102 C SER 1 659	1.103	11.079	10.671	1.00	0.33
ATOM 1103 O SER 1 659	1.317	11.168	9.463	1.00	0.33
ATOM 1104 CB SER 1 659	2.133	12.823	12.043	1.00	0.33
ATOM 1105 OG SER 1 659	3.071	13.105	13.069	1.00	0.33
ATOM 1106 N TYR 1 660	-0.109	10.799	11.175	1.00	0.39
ATOM 1107 CA TYR 1 660	-1.245	10.449	10.377	1.00	0.39
ATOM 1108 C TYR 1 660	-1.494	11.533	9.376	1.00	0.39
ATOM 1109 O TYR 1 660	-1.664	11.257	8.191	1.00	0.39
ATOM 1110 CB TYR 1 660	-2.492	10.287	11.262	1.00	0.39
ATOM 1111 CG TYR 1 660	-3.708	10.080	10.430	1.00	0.39
ATOM 1112 CD1 TYR 1 660	-4.415	11.165	9.970	1.00	0.39
ATOM 1113 CD2 TYR 1 660	-4.142	8.814	10.116	1.00	0.39
ATOM 1114 CE1 TYR 1 660	-5.545	10.989	9.211	1.00	0.39
ATOM 1115 CE2 TYR 1 660	-5.274	8.632	9.356	1.00	0.39
ATOM 1116 CZ TYR 1 660	-5.975	9.723	8.904	1.00	0.39
ATOM 1117 OH TYR 1 660	-7.137	9.553	8.127	1.00	0.39
ATOM 1118 N GLU 1 661	-1.466	12.804	9.817	1.00	0.36
ATOM 1119 CA GLU 1 661	-1.754	13.901	8.938	1.00	0.36
ATOM 1120 C GLU 1 661	-0.746	13.930	7.832	1.00	0.36
ATOM 1121 O GLU 1 661	-1.076	14.301	6.706	1.00	0.36
ATOM 1122 CB GLU 1 661	-1.719	15.268	9.645	1.00	0.36
ATOM 1123 CG GLU 1 661	-2.864	15.467	10.642	1.00	0.36
ATOM 1124 CD GLU 1 661	-2.565	14.634	11.881	1.00	0.36
ATOM 1125 OE1 GLU 1 661	-1.391	14.207	12.038	1.00	0.36
ATOM 1126 OE2 GLU 1 661	-3.508	14.418	12.688	1.00	0.36
ATOM 1127 N GLU 1 662	0.524	13.591	8.133	1.00	0.23
ATOM 1128 CA GLU 1 662	1.551	13.575	7.125	1.00	0.23
ATOM 1129 C GLU 1 662	1.317	12.434	6.184	1.00	0.23
ATOM 1130 O GLU 1 662	1.569	12.533	4.984	1.00	0.23
ATOM 1131 CB GLU 1 662	2.968	13.378	7.687	1.00	0.23
ATOM 1132 CG GLU 1 662	3.493	14.567	8.489	1.00	0.23
ATOM 1133 CD GLU 1 662	4.891	14.209	8.965	1.00	0.23
ATOM 1134 OE1 GLU 1 662	5.669	13.651	8.145	1.00	0.23
ATOM 1135 OE2 GLU 1 662	5.204	14.494	10.151	1.00	0.23
ATOM 1136 N TYR 1 663	0.819	11.313	6.731	1.00	0.31
ATOM 1137 CA TYR 1 663	0.667	10.083	6.013	1.00	0.31

160/208

ATOM	1138	C	TYR	1	663	-0.231	10.312	4.845	1.00	0.31
ATOM	1139	O	TYR	1	663	0.076	9.940	3.710	1.00	0.31
ATOM	1140	CB	TYR	1	663	-0.070	9.047	6.866	1.00	0.31
ATOM	1141	CG	TYR	1	663	0.473	7.805	6.318	1.00	0.31
ATOM	1142	CD1	TYR	1	663	1.757	7.581	6.691	1.00	0.31
ATOM	1143	CD2	TYR	1	663	-0.175	6.941	5.463	1.00	0.31
ATOM	1144	CE1	TYR	1	663	2.411	6.485	6.248	1.00	0.31
ATOM	1145	CE2	TYR	1	663	0.491	5.822	5.012	1.00	0.31
ATOM	1146	CZ	TYR	1	663	1.789	5.609	5.421	1.00	0.31
ATOM	1147	OH	TYR	1	663	2.569	4.512	5.023	1.00	0.31
ATOM	1148	N	LEU	1	664	-1.376	10.951	5.113	1.00	0.36
ATOM	1149	CA	LEU	1	664	-2.358	11.202	4.104	1.00	0.36
ATOM	1150	C	LEU	1	664	-1.794	12.138	3.088	1.00	0.36
ATOM	1151	O	LEU	1	664	-2.156	12.078	1.914	1.00	0.36
ATOM	1152	CB	LEU	1	664	-3.654	11.824	4.650	1.00	0.36
ATOM	1153	CG	LEU	1	664	-4.516	10.837	5.459	1.00	0.36
ATOM	1154	CD1	LEU	1	664	-3.780	10.338	6.710	1.00	0.36
ATOM	1155	CD2	LEU	1	664	-5.896	11.435	5.776	1.00	0.36
ATOM	1156	N	CYS	1	665	-0.926	13.065	3.522	1.00	0.37
ATOM	1157	CA	CYS	1	665	-0.336	13.982	2.594	1.00	0.37
ATOM	1158	C	CYS	1	665	0.482	13.184	1.632	1.00	0.37
ATOM	1159	O	CYS	1	665	0.372	13.358	0.421	1.00	0.37
ATOM	1160	CB	CYS	1	665	0.625	14.981	3.259	1.00	0.37
ATOM	1161	SG	CYS	1	665	-0.212	16.121	4.393	1.00	0.37
ATOM	1162	N	MET	1	666	1.293	12.246	2.154	1.00	0.45
ATOM	1163	CA	MET	1	666	2.172	11.464	1.336	1.00	0.45
ATOM	1164	C	MET	1	666	1.375	10.673	0.347	1.00	0.45
ATOM	1165	O	MET	1	666	1.759	10.575	-0.814	1.00	0.45
ATOM	1166	CB	MET	1	666	3.018	10.467	2.147	1.00	0.45
ATOM	1167	CG	MET	1	666	3.956	9.633	1.274	1.00	0.45
ATOM	1168	SD	MET	1	666	5.010	8.470	2.189	1.00	0.45
ATOM	1169	CE	MET	1	666	6.373	9.637	2.459	1.00	0.45
ATOM	1170	N	LYS	1	667	0.237	10.088	0.757	1.00	0.30
ATOM	1171	CA	LYS	1	667	-0.507	9.286	-0.175	1.00	0.30
ATOM	1172	C	LYS	1	667	-0.958	10.133	-1.326	1.00	0.30
ATOM	1173	O	LYS	1	667	-0.840	9.744	-2.487	1.00	0.30
ATOM	1174	CB	LYS	1	667	-1.785	8.696	0.426	1.00	0.30
ATOM	1175	CG	LYS	1	667	-1.550	7.656	1.515	1.00	0.30
ATOM	1176	CD	LYS	1	667	-2.849	7.288	2.226	1.00	0.30
ATOM	1177	CE	LYS	1	667	-2.758	6.022	3.068	1.00	0.30
ATOM	1178	NZ	LYS	1	667	-4.121	5.496	3.299	1.00	0.30
ATOM	1179	N	THR	1	668	-1.476	11.336	-1.031	1.00	0.20
ATOM	1180	CA	THR	1	668	-1.979	12.209	-2.052	1.00	0.20
ATOM	1181	C	THR	1	668	-0.879	12.491	-3.017	1.00	0.20
ATOM	1182	O	THR	1	668	-1.107	12.489	-4.228	1.00	0.20
ATOM	1183	CB	THR	1	668	-2.402	13.536	-1.484	1.00	0.20
ATOM	1184	OG1	THR	1	668	-3.495	13.371	-0.595	1.00	0.20
ATOM	1185	CG2	THR	1	668	-2.732	14.526	-2.617	1.00	0.20
ATOM	1186	N	LEU	1	669	0.343	12.742	-2.503	1.00	0.37
ATOM	1187	CA	LEU	1	669	1.433	13.036	-3.388	1.00	0.37
ATOM	1188	C	LEU	1	669	1.656	11.861	-4.283	1.00	0.37
ATOM	1189	O	LEU	1	669	1.853	12.038	-5.484	1.00	0.37
ATOM	1190	CB	LEU	1	669	2.822	13.276	-2.742	1.00	0.37
ATOM	1191	CG	LEU	1	669	3.081	14.631	-2.046	1.00	0.37
ATOM	1192	CD1	LEU	1	669	2.497	14.704	-0.634	1.00	0.37
ATOM	1193	CD2	LEU	1	669	4.577	14.979	-2.072	1.00	0.37
ATOM	1194	N	LEU	1	670	1.629	10.629	-3.732	1.00	0.59
ATOM	1195	CA	LEU	1	670	1.882	9.492	-4.572	1.00	0.59
ATOM	1196	C	LEU	1	670	0.874	9.452	-5.663	1.00	0.59
ATOM	1197	O	LEU	1	670	1.230	9.194	-6.811	1.00	0.59
ATOM	1198	CB	LEU	1	670	1.785	8.122	-3.883	1.00	0.59

161/208

ATOM 1199	CG LEU 1 670	3.047	7.742	-3.111	1.00	0.59
ATOM 1200	CD1 LEU 1 670	4.214	7.424	-4.058	1.00	0.59
ATOM 1201	CD2 LEU 1 670	3.402	8.843	-2.123	1.00	0.59
ATOM 1202	N LEU 1 671	-0.409	9.705	-5.340	1.00	0.65
ATOM 1203	CA LEU 1 671	-1.397	9.629	-6.375	1.00	0.65
ATOM 1204	C LEU 1 671	-1.038	10.568	-7.470	1.00	0.65
ATOM 1205	O LEU 1 671	-0.835	10.166	-8.610	1.00	0.65
ATOM 1206	CB LEU 1 671	-2.799	10.126	-5.970	1.00	0.65
ATOM 1207	CG LEU 1 671	-3.703	9.172	-5.185	1.00	0.65
ATOM 1208	CD1 LEU 1 671	-5.038	9.852	-4.883	1.00	0.65
ATOM 1209	CD2 LEU 1 671	-3.954	7.872	-5.951	1.00	0.65
ATOM 1210	N LEU 1 672	-0.900	11.852	-7.135	1.00	0.38
ATOM 1211	CA LEU 1 672	-0.726	12.829	-8.161	1.00	0.38
ATOM 1212	C LEU 1 672	0.607	12.768	-8.850	1.00	0.38
ATOM 1213	O LEU 1 672	0.650	13.085	-10.033	1.00	0.38
ATOM 1214	CB LEU 1 672	-1.020	14.240	-7.643	1.00	0.38
ATOM 1215	CG LEU 1 672	-2.500	14.386	-7.248	1.00	0.38
ATOM 1216	CD1 LEU 1 672	-2.818	15.790	-6.727	1.00	0.38
ATOM 1217	CD2 LEU 1 672	-3.419	13.962	-8.403	1.00	0.38
ATOM 1218	N SER 1 673	1.705	12.430	-8.134	1.00	0.29
ATOM 1219	CA SER 1 673	3.082	12.426	-8.596	1.00	0.29
ATOM 1220	C SER 1 673	3.549	11.254	-9.428	1.00	0.29
ATOM 1221	O SER 1 673	4.437	11.413	-10.265	1.00	0.29
ATOM 1222	CB SER 1 673	4.077	12.541	-7.428	1.00	0.29
ATOM 1223	OG SER 1 673	5.410	12.535	-7.921	1.00	0.29
ATOM 1224	N SER 1 674	3.027	10.038	-9.221	1.00	0.48
ATOM 1225	CA SER 1 674	3.583	8.903	-9.911	1.00	0.48
ATOM 1226	C SER 1 674	3.374	8.971	-11.400	1.00	0.48
ATOM 1227	O SER 1 674	4.267	8.606	-12.161	1.00	0.48
ATOM 1228	CB SER 1 674	2.982	7.579	-9.435	1.00	0.48
ATOM 1229	OG SER 1 674	1.642	7.481	-9.888	1.00	0.48
ATOM 1230	N VAL 1 675	2.190	9.408	-11.869	1.00	0.57
ATOM 1231	CA VAL 1 675	1.945	9.412	-13.290	1.00	0.57
ATOM 1232	C VAL 1 675	1.945	10.799	-13.936	1.00	0.57
ATOM 1233	O VAL 1 675	1.416	10.900	-15.043	1.00	0.57
ATOM 1234	CB VAL 1 675	0.635	8.762	-13.627	1.00	0.57
ATOM 1235	CG1 VAL 1 675	-0.491	9.748	-13.281	1.00	0.57
ATOM 1236	CG2 VAL 1 675	0.655	8.272	-15.086	1.00	0.57
ATOM 1237	N PRO 1 676	2.488	11.888	-13.439	1.00	0.65
ATOM 1238	CA PRO 1 676	2.417	13.095	-14.211	1.00	0.65
ATOM 1239	C PRO 1 676	3.203	13.051	-15.468	1.00	0.65
ATOM 1240	O PRO 1 676	2.954	13.897	-16.323	1.00	0.65
ATOM 1241	CB PRO 1 676	2.950	14.214	-13.339	1.00	0.65
ATOM 1242	CG PRO 1 676	2.582	13.762	-11.938	1.00	0.65
ATOM 1243	CD PRO 1 676	2.432	12.239	-12.039	1.00	0.65
ATOM 1244	N LYS 1 677	4.169	12.127	-15.600	1.00	0.81
ATOM 1245	CA LYS 1 677	4.988	12.215	-16.772	1.00	0.81
ATOM 1246	C LYS 1 677	4.357	11.485	-17.906	1.00	0.81
ATOM 1247	O LYS 1 677	5.035	10.801	-18.672	1.00	0.81
ATOM 1248	CB LYS 1 677	6.414	11.670	-16.591	1.00	0.81
ATOM 1249	CG LYS 1 677	6.511	10.152	-16.450	1.00	0.81
ATOM 1250	CD LYS 1 677	7.937	9.637	-16.666	1.00	0.81
ATOM 1251	CE LYS 1 677	8.078	8.121	-16.535	1.00	0.81
ATOM 1252	NZ LYS 1 677	9.482	7.727	-16.788	1.00	0.81
ATOM 1253	N ASP 1 678	3.030	11.611	-18.057	1.00	0.80
ATOM 1254	CA ASP 1 678	2.404	11.004	-19.187	1.00	0.80
ATOM 1255	C ASP 1 678	1.320	11.940	-19.604	1.00	0.80
ATOM 1256	O ASP 1 678	0.978	12.874	-18.882	1.00	0.80
ATOM 1257	CB ASP 1 678	1.746	9.646	-18.885	1.00	0.80
ATOM 1258	CG ASP 1 678	2.859	8.628	-18.686	1.00	0.80
ATOM 1259	OD1 ASP 1 678	3.855	8.684	-19.456	1.00	0.80

162/208

ATOM	1260	OD2 ASP 1 678	2.726	7.775	-17.767	1.00	0.80
ATOM	1261	N GLY 1 679	0.778	11.730	-20.816	1.00	0.77
ATOM	1262	CA GLY 1 679	-0.315	12.523	-21.302	1.00	0.77
ATOM	1263	C GLY 1 679	0.169	13.900	-21.640	1.00	0.77
ATOM	1264	O GLY 1 679	0.890	14.513	-20.858	1.00	0.77
ATOM	1265	N LEU 1 680	-0.158	14.402	-22.851	1.00	1.01
ATOM	1266	CA LEU 1 680	0.175	15.758	-23.203	1.00	1.01
ATOM	1267	C LEU 1 680	-0.728	16.705	-22.482	1.00	1.01
ATOM	1268	O LEU 1 680	-0.252	17.616	-21.805	1.00	1.01
ATOM	1269	CB LEU 1 680	0.021	16.043	-24.713	1.00	1.01
ATOM	1270	CG LEU 1 680	0.318	17.497	-25.160	1.00	1.01
ATOM	1271	CD1 LEU 1 680	-0.825	18.473	-24.825	1.00	1.01
ATOM	1272	CD2 LEU 1 680	1.670	17.981	-24.612	1.00	1.01
ATOM	1273	N LYS 1 681	-2.053	16.438	-22.600	1.00	1.15
ATOM	1274	CA LYS 1 681	-3.194	17.213	-22.173	1.00	1.15
ATOM	1275	C LYS 1 681	-2.806	18.505	-21.555	1.00	1.15
ATOM	1276	O LYS 1 681	-3.104	18.782	-20.396	1.00	1.15
ATOM	1277	CB LYS 1 681	-4.149	16.469	-21.217	1.00	1.15
ATOM	1278	CG LYS 1 681	-5.363	17.294	-20.764	1.00	1.15
ATOM	1279	CD LYS 1 681	-6.308	17.721	-21.892	1.00	1.15
ATOM	1280	CE LYS 1 681	-5.970	19.085	-22.502	1.00	1.15
ATOM	1281	NZ LYS 1 681	-6.934	19.413	-23.578	1.00	1.15
ATOM	1282	N SER 1 682	-2.145	19.337	-22.371	1.00	1.05
ATOM	1283	CA SER 1 682	-1.702	20.644	-22.022	1.00	1.05
ATOM	1284	C SER 1 682	-0.818	20.681	-20.819	1.00	1.05
ATOM	1285	O SER 1 682	-0.938	19.922	-19.859	1.00	1.05
ATOM	1286	CB SER 1 682	-2.842	21.658	-21.831	1.00	1.05
ATOM	1287	OG SER 1 682	-2.302	22.944	-21.572	1.00	1.05
ATOM	1288	N GLN 1 683	0.158	21.601	-20.869	1.00	0.99
ATOM	1289	CA GLN 1 683	0.986	21.803	-19.729	1.00	0.99
ATOM	1290	C GLN 1 683	0.069	22.382	-18.708	1.00	0.99
ATOM	1291	O GLN 1 683	0.325	22.312	-17.509	1.00	0.99
ATOM	1292	CB GLN 1 683	2.164	22.774	-19.941	1.00	0.99
ATOM	1293	CG GLN 1 683	1.767	24.207	-20.292	1.00	0.99
ATOM	1294	CD GLN 1 683	1.612	24.282	-21.802	1.00	0.99
ATOM	1295	OE1 GLN 1 683	1.650	23.263	-22.491	1.00	0.99
ATOM	1296	NE2 GLN 1 683	1.440	25.520	-22.335	1.00	0.99
ATOM	1297	N GLU 1 684	-1.033	22.982	-19.192	1.00	0.75
ATOM	1298	CA GLU 1 684	-2.011	23.633	-18.374	1.00	0.75
ATOM	1299	C GLU 1 684	-2.541	22.635	-17.391	1.00	0.75
ATOM	1300	O GLU 1 684	-2.633	22.918	-16.198	1.00	0.75
ATOM	1301	CB GLU 1 684	-3.209	24.109	-19.213	1.00	0.75
ATOM	1302	CG GLU 1 684	-3.940	25.323	-18.649	1.00	0.75
ATOM	1303	CD GLU 1 684	-3.232	26.542	-19.221	1.00	0.75
ATOM	1304	OE1 GLU 1 684	-2.717	26.434	-20.366	1.00	0.75
ATOM	1305	OE2 GLU 1 684	-3.192	27.592	-18.527	1.00	0.75
ATOM	1306	N LEU 1 685	-2.901	21.428	-17.867	1.00	0.40
ATOM	1307	CA LEU 1 685	-3.422	20.422	-16.986	1.00	0.40
ATOM	1308	C LEU 1 685	-2.344	20.017	-16.029	1.00	0.40
ATOM	1309	O LEU 1 685	-2.601	19.817	-14.844	1.00	0.40
ATOM	1310	CB LEU 1 685	-3.924	19.177	-17.735	1.00	0.40
ATOM	1311	CG LEU 1 685	-5.213	19.443	-18.538	1.00	0.40
ATOM	1312	CD1 LEU 1 685	-6.401	19.716	-17.603	1.00	0.40
ATOM	1313	CD2 LEU 1 685	-5.014	20.567	-19.569	1.00	0.40
ATOM	1314	N PHE 1 686	-1.094	19.908	-16.519	1.00	0.20
ATOM	1315	CA PHE 1 686	-0.004	19.513	-15.673	1.00	0.20
ATOM	1316	C PHE 1 686	0.119	20.522	-14.590	1.00	0.20
ATOM	1317	O PHE 1 686	0.333	20.181	-13.429	1.00	0.20
ATOM	1318	CB PHE 1 686	1.374	19.552	-16.353	1.00	0.20
ATOM	1319	CG PHE 1 686	1.516	18.437	-17.319	1.00	0.20
ATOM	1320	CD1 PHE 1 686	1.108	18.581	-18.622	1.00	0.20

163/208

ATOM	1321	CD2 PHE 1 686	2.074	17.251	-16.908	1.00	0.20
ATOM	1322	CE1 PHE 1 686	1.252	17.545	-19.510	1.00	0.20
ATOM	1323	CE2 PHE 1 686	2.221	16.209	-17.786	1.00	0.20
ATOM	1324	CZ PHE 1 686	1.811	16.365	-19.085	1.00	0.20
ATOM	1325	N ASP 1 687	-0.023	21.803	-14.961	1.00	0.18
ATOM	1326	CA ASP 1 687	0.161	22.880	-14.041	1.00	0.18
ATOM	1327	C ASP 1 687	-0.821	22.719	-12.931	1.00	0.18
ATOM	1328	O ASP 1 687	-0.471	22.872	-11.761	1.00	0.18
ATOM	1329	CB ASP 1 687	-0.105	24.251	-14.688	1.00	0.18
ATOM	1330	CG ASP 1 687	0.351	25.336	-13.726	1.00	0.18
ATOM	1331	OD1 ASP 1 687	1.266	25.055	-12.907	1.00	0.18
ATOM	1332	OD2 ASP 1 687	-0.219	26.458	-13.789	1.00	0.18
ATOM	1333	N GLU 1 688	-2.072	22.360	-13.266	1.00	0.34
ATOM	1334	CA GLU 1 688	-3.077	22.276	-12.249	1.00	0.34
ATOM	1335	C GLU 1 688	-2.642	21.283	-11.225	1.00	0.34
ATOM	1336	O GLU 1 688	-2.756	21.530	-10.026	1.00	0.34
ATOM	1337	CB GLU 1 688	-4.446	21.820	-12.785	1.00	0.34
ATOM	1338	CG GLU 1 688	-5.126	22.848	-13.690	1.00	0.34
ATOM	1339	CD GLU 1 688	-6.457	22.266	-14.139	1.00	0.34
ATOM	1340	OE1 GLU 1 688	-6.749	21.099	-13.761	1.00	0.34
ATOM	1341	OE2 GLU 1 688	-7.202	22.977	-14.864	1.00	0.34
ATOM	1342	N ILE 1 689	-2.134	20.120	-11.661	1.00	0.52
ATOM	1343	CA ILE 1 689	-1.692	19.186	-10.674	1.00	0.52
ATOM	1344	C ILE 1 689	-0.476	19.711	-9.981	1.00	0.52
ATOM	1345	O ILE 1 689	-0.302	19.488	-8.787	1.00	0.52
ATOM	1346	CB ILE 1 689	-1.580	17.763	-11.167	1.00	0.52
ATOM	1347	CG1 ILE 1 689	-0.713	17.619	-12.424	1.00	0.52
ATOM	1348	CG2 ILE 1 689	-3.007	17.219	-11.322	1.00	0.52
ATOM	1349	CD1 ILE 1 689	-0.618	16.168	-12.902	1.00	0.52
ATOM	1350	N ARG 1 690	0.375	20.475	-10.685	1.00	0.58
ATOM	1351	CA ARG 1 690	1.570	21.000	-10.086	1.00	0.58
ATOM	1352	C ARG 1 690	1.205	21.876	-8.919	1.00	0.58
ATOM	1353	O ARG 1 690	1.872	21.838	-7.887	1.00	0.58
ATOM	1354	CB ARG 1 690	2.395	21.846	-11.073	1.00	0.58
ATOM	1355	CG ARG 1 690	2.876	21.049	-12.289	1.00	0.58
ATOM	1356	CD ARG 1 690	3.698	21.869	-13.287	1.00	0.58
ATOM	1357	NE ARG 1 690	5.061	22.037	-12.708	1.00	0.58
ATOM	1358	CZ ARG 1 690	6.127	22.282	-13.526	1.00	0.58
ATOM	1359	NH1 ARG 1 690	5.949	22.370	-14.877	1.00	0.58
ATOM	1360	NH2 ARG 1 690	7.373	22.439	-12.991	1.00	0.58
ATOM	1361	N MET 1 691	0.148	22.704	-9.052	1.00	0.57
ATOM	1362	CA MET 1 691	-0.257	23.562	-7.971	1.00	0.57
ATOM	1363	C MET 1 691	-0.751	22.736	-6.830	1.00	0.57
ATOM	1364	O MET 1 691	-0.517	23.066	-5.668	1.00	0.57
ATOM	1365	CB MET 1 691	-1.405	24.534	-8.307	1.00	0.57
ATOM	1366	CG MET 1 691	-1.007	25.800	-9.067	1.00	0.57
ATOM	1367	SD MET 1 691	-0.638	25.574	-10.827	1.00	0.57
ATOM	1368	CE MET 1 691	-0.327	27.335	-11.148	1.00	0.57
ATOM	1369	N THR 1 692	-1.487	21.649	-7.108	1.00	0.47
ATOM	1370	CA THR 1 692	-1.976	20.900	-5.993	1.00	0.47
ATOM	1371	C THR 1 692	-0.798	20.310	-5.283	1.00	0.47
ATOM	1372	O THR 1 692	-0.778	20.269	-4.052	1.00	0.47
ATOM	1373	CB THR 1 692	-2.930	19.795	-6.349	1.00	0.47
ATOM	1374	OG1 THR 1 692	-3.587	19.327	-5.181	1.00	0.47
ATOM	1375	CG2 THR 1 692	-2.147	18.640	-6.976	1.00	0.47
ATOM	1376	N TYR 1 693	0.229	19.855	-6.039	1.00	0.41
ATOM	1377	CA TYR 1 693	1.366	19.242	-5.406	1.00	0.41
ATOM	1378	C TYR 1 693	1.979	20.255	-4.506	1.00	0.41
ATOM	1379	O TYR 1 693	2.279	19.971	-3.347	1.00	0.41
ATOM	1380	CB TYR 1 693	2.564	18.873	-6.316	1.00	0.41
ATOM	1381	CG TYR 1 693	2.140	18.002	-7.437	1.00	0.41

164/208

ATOM	1382	CD1 TYR 1 693	1.664	16.735	-7.211	1.00	0.41
ATOM	1383	CD2 TYR 1 693	2.219	18.473	-8.724	1.00	0.41
ATOM	1384	CE1 TYR 1 693	1.261	15.968	-8.273	1.00	0.41
ATOM	1385	CE2 TYR 1 693	1.814	17.709	-9.788	1.00	0.41
ATOM	1386	CZ TYR 1 693	1.330	16.449	-9.554	1.00	0.41
ATOM	1387	OH TYR 1 693	0.901	15.648	-10.626	1.00	0.41
ATOM	1388	N ILE 1 694	2.176	21.482	-5.022	1.00	0.49
ATOM	1389	CA ILE 1 694	2.828	22.476	-4.228	1.00	0.49
ATOM	1390	C ILE 1 694	1.964	22.742	-3.047	1.00	0.49
ATOM	1391	O ILE 1 694	2.454	22.994	-1.949	1.00	0.49
ATOM	1392	CB ILE 1 694	3.091	23.776	-4.943	1.00	0.49
ATOM	1393	CG1 ILE 1 694	4.098	24.616	-4.141	1.00	0.49
ATOM	1394	CG2 ILE 1 694	1.758	24.501	-5.174	1.00	0.49
ATOM	1395	CD1 ILE 1 694	5.495	24.000	-4.085	1.00	0.49
ATOM	1396	N LYS 1 695	0.636	22.677	-3.244	1.00	0.48
ATOM	1397	CA LYS 1 695	-0.261	22.939	-2.163	1.00	0.48
ATOM	1398	C LYS 1 695	-0.026	21.937	-1.074	1.00	0.48
ATOM	1399	O LYS 1 695	0.007	22.294	0.103	1.00	0.48
ATOM	1400	CB LYS 1 695	-1.731	22.841	-2.580	1.00	0.48
ATOM	1401	CG LYS 1 695	-2.652	23.125	-1.404	1.00	0.48
ATOM	1402	CD LYS 1 695	-4.097	23.419	-1.775	1.00	0.48
ATOM	1403	CE LYS 1 695	-4.909	23.685	-0.516	1.00	0.48
ATOM	1404	NZ LYS 1 695	-4.012	24.318	0.480	1.00	0.48
ATOM	1405	N GLU 1 696	0.150	20.653	-1.435	1.00	0.53
ATOM	1406	CA GLU 1 696	0.333	19.620	-0.456	1.00	0.53
ATOM	1407	C GLU 1 696	1.620	19.825	0.281	1.00	0.53
ATOM	1408	O GLU 1 696	1.708	19.539	1.474	1.00	0.53
ATOM	1409	CB GLU 1 696	0.324	18.217	-1.073	1.00	0.53
ATOM	1410	CG GLU 1 696	0.482	17.109	-0.039	1.00	0.53
ATOM	1411	CD GLU 1 696	-0.216	15.890	-0.609	1.00	0.53
ATOM	1412	OE1 GLU 1 696	0.118	15.476	-1.754	1.00	0.53
ATOM	1413	OE2 GLU 1 696	-1.124	15.376	0.094	1.00	0.53
ATOM	1414	N LEU 1 697	2.664	20.309	-0.413	1.00	0.53
ATOM	1415	CA LEU 1 697	3.923	20.528	0.235	1.00	0.53
ATOM	1416	C LEU 1 697	3.675	21.553	1.294	1.00	0.53
ATOM	1417	O LEU 1 697	4.124	21.409	2.431	1.00	0.53
ATOM	1418	CB LEU 1 697	4.979	21.072	-0.754	1.00	0.53
ATOM	1419	CG LEU 1 697	6.432	21.204	-0.237	1.00	0.53
ATOM	1420	CD1 LEU 1 697	7.343	21.760	-1.342	1.00	0.53
ATOM	1421	CD2 LEU 1 697	6.556	22.030	1.052	1.00	0.53
ATOM	1422	N GLY 1 698	2.918	22.610	0.947	1.00	0.46
ATOM	1423	CA GLY 1 698	2.678	23.669	1.882	1.00	0.46
ATOM	1424	C GLY 1 698	2.004	23.090	3.082	1.00	0.46
ATOM	1425	O GLY 1 698	2.368	23.403	4.215	1.00	0.46
ATOM	1426	N LYS 1 699	1.007	22.213	2.863	1.00	0.51
ATOM	1427	CA LYS 1 699	0.292	21.641	3.965	1.00	0.51
ATOM	1428	C LYS 1 699	1.257	20.845	4.780	1.00	0.51
ATOM	1429	O LYS 1 699	1.223	20.891	6.008	1.00	0.51
ATOM	1430	CB LYS 1 699	-0.839	20.695	3.531	1.00	0.51
ATOM	1431	CG LYS 1 699	-1.677	20.116	4.678	1.00	0.51
ATOM	1432	CD LYS 1 699	-0.960	19.104	5.576	1.00	0.51
ATOM	1433	CE LYS 1 699	-1.900	18.336	6.503	1.00	0.51
ATOM	1434	NZ LYS 1 699	-2.649	17.334	5.716	1.00	0.51
ATOM	1435	N ALA 1 700	2.147	20.088	4.116	1.00	0.30
ATOM	1436	CA ALA 1 700	3.064	19.273	4.856	1.00	0.30
ATOM	1437	C ALA 1 700	3.878	20.181	5.719	1.00	0.30
ATOM	1438	O ALA 1 700	4.070	19.912	6.901	1.00	0.30
ATOM	1439	CB ALA 1 700	4.032	18.493	3.951	1.00	0.30
ATOM	1440	N ILE 1 701	4.363	21.300	5.154	1.00	0.10
ATOM	1441	CA ILE 1 701	5.161	22.196	5.940	1.00	0.10
ATOM	1442	C ILE 1 701	4.318	22.798	7.019	1.00	0.10

165/208

ATOM 1443 O ILE 1 701	4.811	23.027	8.119	1.00	0.10
ATOM 1444 CB ILE 1 701	5.779	23.316	5.157	1.00	0.10
ATOM 1445 CG1 ILE 1 701	6.800	22.756	4.156	1.00	0.10
ATOM 1446 CG2 ILE 1 701	6.380	24.319	6.154	1.00	0.10
ATOM 1447 CD1 ILE 1 701	7.389	23.822	3.239	1.00	0.10
ATOM 1448 N VAL 1 702	3.027	23.067	6.751	1.00	0.25
ATOM 1449 CA VAL 1 702	2.179	23.698	7.728	1.00	0.25
ATOM 1450 C VAL 1 702	2.105	22.838	8.953	1.00	0.25
ATOM 1451 O VAL 1 702	2.160	23.345	10.074	1.00	0.25
ATOM 1452 CB VAL 1 702	0.773	23.893	7.237	1.00	0.25
ATOM 1453 CG1 VAL 1 702	-0.072	24.462	8.390	1.00	0.25
ATOM 1454 CG2 VAL 1 702	0.804	24.793	5.992	1.00	0.25
ATOM 1455 N LYS 1 703	1.976	21.510	8.782	1.00	0.54
ATOM 1456 CA LYS 1 703	1.907	20.638	9.921	1.00	0.54
ATOM 1457 C LYS 1 703	3.202	20.763	10.655	1.00	0.54
ATOM 1458 O LYS 1 703	3.252	20.709	11.882	1.00	0.54
ATOM 1459 CB LYS 1 703	1.736	19.156	9.544	1.00	0.54
ATOM 1460 CG LYS 1 703	0.302	18.767	9.175	1.00	0.54
ATOM 1461 CD LYS 1 703	-0.678	18.913	10.343	1.00	0.54
ATOM 1462 CE LYS 1 703	-2.115	18.520	9.997	1.00	0.54
ATOM 1463 NZ LYS 1 703	-2.697	19.497	9.051	1.00	0.54
ATOM 1464 N ARG 1 704	4.285	20.916	9.876	1.00	0.56
ATOM 1465 CA ARG 1 704	5.649	21.052	10.296	1.00	0.56
ATOM 1466 C ARG 1 704	5.826	22.375	10.975	1.00	0.56
ATOM 1467 O ARG 1 704	6.790	22.569	11.706	1.00	0.56
ATOM 1468 CB ARG 1 704	6.621	21.060	9.110	1.00	0.56
ATOM 1469 CG ARG 1 704	6.476	19.841	8.203	1.00	0.56
ATOM 1470 CD ARG 1 704	7.538	18.769	8.399	1.00	0.56
ATOM 1471 NE ARG 1 704	7.227	17.677	7.435	1.00	0.56
ATOM 1472 CZ ARG 1 704	7.577	17.824	6.126	1.00	0.56
ATOM 1473 NH1 ARG 1 704	8.094	19.016	5.707	1.00	0.56
ATOM 1474 NH2 ARG 1 704	7.393	16.800	5.241	1.00	0.56
ATOM 1475 N GLU 1 705	4.943	23.351	10.703	1.00	0.33
ATOM 1476 CA GLU 1 705	5.067	24.660	11.273	1.00	0.33
ATOM 1477 C GLU 1 705	5.018	24.487	12.745	1.00	0.33
ATOM 1478 O GLU 1 705	5.553	25.308	13.487	1.00	0.33
ATOM 1479 CB GLU 1 705	3.927	25.610	10.865	1.00	0.33
ATOM 1480 CG GLU 1 705	3.971	26.009	9.388	1.00	0.33
ATOM 1481 CD GLU 1 705	2.801	26.945	9.116	1.00	0.33
ATOM 1482 OE1 GLU 1 705	1.661	26.599	9.526	1.00	0.33
ATOM 1483 OE2 GLU 1 705	3.033	28.020	8.502	1.00	0.33
ATOM 1484 N GLY 1 706	4.349	23.411	13.199	1.00	0.32
ATOM 1485 CA GLY 1 706	4.308	23.157	14.606	1.00	0.32
ATOM 1486 C GLY 1 706	5.740	23.077	15.057	1.00	0.32
ATOM 1487 O GLY 1 706	6.110	23.626	16.093	1.00	0.32
ATOM 1488 N ASN 1 707	6.583	22.380	14.269	1.00	0.57
ATOM 1489 CA ASN 1 707	8.003	22.293	14.495	1.00	0.57
ATOM 1490 C ASN 1 707	8.678	23.518	13.914	1.00	0.57
ATOM 1491 O ASN 1 707	8.123	24.615	13.978	1.00	0.57
ATOM 1492 CB ASN 1 707	8.675	21.053	13.883	1.00	0.57
ATOM 1493 CG ASN 1 707	8.450	19.896	14.845	1.00	0.57
ATOM 1494 OD1 ASN 1 707	8.562	20.061	16.059	1.00	0.57
ATOM 1495 ND2 ASN 1 707	8.128	18.695	14.295	1.00	0.57
ATOM 1496 N SER 1 708	9.913	23.381	13.351	1.00	0.75
ATOM 1497 CA SER 1 708	10.585	24.562	12.856	1.00	0.75
ATOM 1498 C SER 1 708	11.409	24.261	11.624	1.00	0.75
ATOM 1499 O SER 1 708	10.923	23.649	10.675	1.00	0.75
ATOM 1500 CB SER 1 708	11.518	25.203	13.903	1.00	0.75
ATOM 1501 OG SER 1 708	11.979	26.472	13.456	1.00	0.75
ATOM 1502 N SER 1 709	12.701	24.680	11.637	1.00	0.78
ATOM 1503 CA SER 1 709	13.639	24.623	10.539	1.00	0.78

166/208

ATOM	1504	C	SER	1709	13.812	23.206	10.131	1.00	0.78
ATOM	1505	O	SER	1709	14.038	22.890	8.963	1.00	0.78
ATOM	1506	CB	SER	1709	15.027	25.173	10.906	1.00	0.78
ATOM	1507	OG	SER	1709	15.895	25.089	9.785	1.00	0.78
ATOM	1508	N	GLN	1710	13.662	22.297	11.097	1.00	0.75
ATOM	1509	CA	GLN	1710	13.776	20.896	10.850	1.00	0.75
ATOM	1510	C	GLN	1710	12.756	20.537	9.812	1.00	0.75
ATOM	1511	O	GLN	1710	12.848	19.490	9.176	1.00	0.75
ATOM	1512	CB	GLN	1710	13.556	20.062	12.126	1.00	0.75
ATOM	1513	CG	GLN	1710	12.186	20.243	12.786	1.00	0.75
ATOM	1514	CD	GLN	1710	11.210	19.233	12.201	1.00	0.75
ATOM	1515	OE1	GLN	1710	10.623	19.439	11.140	1.00	0.75
ATOM	1516	NE2	GLN	1710	11.024	18.097	12.925	1.00	0.75
ATOM	1517	N	ASN	1711	11.739	21.396	9.614	1.00	0.76
ATOM	1518	CA	ASN	1711	10.693	21.096	8.687	1.00	0.76
ATOM	1519	C	ASN	1711	11.273	20.783	7.340	1.00	0.76
ATOM	1520	O	ASN	1711	10.878	19.797	6.721	1.00	0.76
ATOM	1521	CB	ASN	1711	9.669	22.243	8.500	1.00	0.76
ATOM	1522	CG	ASN	1711	10.266	23.392	7.691	1.00	0.76
ATOM	1523	OD1	ASN	1711	9.671	23.816	6.701	1.00	0.76
ATOM	1524	ND2	ASN	1711	11.464	23.898	8.088	1.00	0.76
ATOM	1525	N	TRP	1712	12.239	21.579	6.841	1.00	0.75
ATOM	1526	CA	TRP	1712	12.723	21.288	5.526	1.00	0.75
ATOM	1527	C	TRP	1712	13.425	19.976	5.555	1.00	0.75
ATOM	1528	O	TRP	1712	13.300	19.181	4.626	1.00	0.75
ATOM	1529	CB	TRP	1712	13.655	22.361	4.925	1.00	0.75
ATOM	1530	CG	TRP	1712	14.940	22.648	5.661	1.00	0.75
ATOM	1531	CD1	TRP	1712	15.209	23.608	6.592	1.00	0.75
ATOM	1532	CD2	TRP	1712	16.165	21.927	5.457	1.00	0.75
ATOM	1533	NE1	TRP	1712	16.525	23.530	6.981	1.00	0.75
ATOM	1534	CE2	TRP	1712	17.126	22.501	6.289	1.00	0.75
ATOM	1535	CE3	TRP	1712	16.465	20.877	4.637	1.00	0.75
ATOM	1536	CZ2	TRP	1712	18.406	22.030	6.315	1.00	0.75
ATOM	1537	CZ3	TRP	1712	17.757	20.402	4.669	1.00	0.75
ATOM	1538	CH2	TRP	1712	18.710	20.967	5.492	1.00	0.75
ATOM	1539	N	GLN	1713	14.177	19.695	6.634	1.00	0.74
ATOM	1540	CA	GLN	1713	14.891	18.457	6.634	1.00	0.74
ATOM	1541	C	GLN	1713	13.930	17.308	6.637	1.00	0.74
ATOM	1542	O	GLN	1713	14.136	16.347	5.898	1.00	0.74
ATOM	1543	CB	GLN	1713	15.880	18.271	7.805	1.00	0.74
ATOM	1544	CG	GLN	1713	15.253	18.190	9.195	1.00	0.74
ATOM	1545	CD	GLN	1713	16.378	18.001	10.202	1.00	0.74
ATOM	1546	OE1	GLN	1713	17.241	17.142	10.026	1.00	0.74
ATOM	1547	NE2	GLN	1713	16.375	18.824	11.285	1.00	0.74
ATOM	1548	N	ARG	1714	12.852	17.354	7.452	1.00	0.79
ATOM	1549	CA	ARG	1714	12.025	16.180	7.441	1.00	0.79
ATOM	1550	C	ARG	1714	11.270	16.111	6.153	1.00	0.79
ATOM	1551	O	ARG	1714	10.972	15.018	5.677	1.00	0.79
ATOM	1552	CB	ARG	1714	11.013	15.980	8.582	1.00	0.79
ATOM	1553	CG	ARG	1714	9.787	16.880	8.603	1.00	0.79
ATOM	1554	CD	ARG	1714	8.678	16.232	9.436	1.00	0.79
ATOM	1555	NE	ARG	1714	8.479	14.866	8.866	1.00	0.79
ATOM	1556	CZ	ARG	1714	8.281	13.792	9.687	1.00	0.79
ATOM	1557	NH1	ARG	1714	8.141	13.974	11.032	1.00	0.79
ATOM	1558	NH2	ARG	1714	8.236	12.531	9.163	1.00	0.79
ATOM	1559	N	PHE	1715	10.938	17.275	5.557	1.00	0.65
ATOM	1560	CA	PHE	1715	10.213	17.296	4.317	1.00	0.65
ATOM	1561	C	PHE	1715	10.983	16.458	3.352	1.00	0.65
ATOM	1562	O	PHE	1715	10.428	15.591	2.677	1.00	0.65
ATOM	1563	CB	PHE	1715	10.144	18.722	3.732	1.00	0.65
ATOM	1564	CG	PHE	1715	9.605	18.677	2.343	1.00	0.65



167/208

ATOM 1565	CD1 PHE 1 715	10.456	18.485	1.279	1.00	0.65
ATOM 1566	CD2 PHE 1 715	8.261	18.839	2.098	1.00	0.65
ATOM 1567	CE1 PHE 1 715	9.980	18.442	-0.009	1.00	0.65
ATOM 1568	CE2 PHE 1 715	7.778	18.796	0.810	1.00	0.65
ATOM 1569	CZ PHE 1 715	8.636	18.600	-0.245	1.00	0.65
ATOM 1570	N TYR 1 716	12.304	16.684	3.293	1.00	0.39
ATOM 1571	CA TYR 1 716	13.139	15.973	2.374	1.00	0.39
ATOM 1572	C TYR 1 716	13.190	14.523	2.758	1.00	0.39
ATOM 1573	O TYR 1 716	13.166	13.645	1.898	1.00	0.39
ATOM 1574	CB TYR 1 716	14.574	16.527	2.358	1.00	0.39
ATOM 1575	CG TYR 1 716	15.270	15.962	1.170	1.00	0.39
ATOM 1576	CD1 TYR 1 716	14.998	16.459	-0.084	1.00	0.39
ATOM 1577	CD2 TYR 1 716	16.199	14.958	1.303	1.00	0.39
ATOM 1578	CE1 TYR 1 716	15.632	15.958	-1.196	1.00	0.39
ATOM 1579	CE2 TYR 1 716	16.835	14.453	0.193	1.00	0.39
ATOM 1580	CZ TYR 1 716	16.553	14.949	-1.057	1.00	0.39
ATOM 1581	OH TYR 1 716	17.210	14.426	-2.192	1.00	0.39
ATOM 1582	N GLN 1 717	13.246	14.226	4.069	1.00	0.36
ATOM 1583	CA GLN 1 717	13.376	12.867	4.515	1.00	0.36
ATOM 1584	C GLN 1 717	12.169	12.094	4.088	1.00	0.36
ATOM 1585	O GLN 1 717	12.266	10.940	3.674	1.00	0.36
ATOM 1586	CB GLN 1 717	13.486	12.774	6.047	1.00	0.36
ATOM 1587	CG GLN 1 717	14.732	13.473	6.595	1.00	0.36
ATOM 1588	CD GLN 1 717	14.729	13.344	8.112	1.00	0.36
ATOM 1589	OE1 GLN 1 717	13.812	12.773	8.699	1.00	0.36
ATOM 1590	NE2 GLN 1 717	15.784	13.899	8.767	1.00	0.36
ATOM 1591	N LEU 1 718	10.995	12.730	4.195	1.00	0.57
ATOM 1592	CA LEU 1 718	9.732	12.125	3.904	1.00	0.57
ATOM 1593	C LEU 1 718	9.666	11.818	2.429	1.00	0.57
ATOM 1594	O LEU 1 718	9.368	10.690	2.038	1.00	0.57
ATOM 1595	CB LEU 1 718	8.641	13.110	4.380	1.00	0.57
ATOM 1596	CG LEU 1 718	7.234	12.552	4.638	1.00	0.57
ATOM 1597	CD1 LEU 1 718	6.404	12.443	3.364	1.00	0.57
ATOM 1598	CD2 LEU 1 718	7.308	11.232	5.423	1.00	0.57
ATOM 1599	N THR 1 719	10.036	12.791	1.569	1.00	0.57
ATOM 1600	CA THR 1 719	9.946	12.619	0.142	1.00	0.57
ATOM 1601	C THR 1 719	10.827	11.486	-0.296	1.00	0.57
ATOM 1602	O THR 1 719	10.443	10.696	-1.157	1.00	0.57
ATOM 1603	CB THR 1 719	10.346	13.839	-0.634	1.00	0.57
ATOM 1604	OG1 THR 1 719	10.019	13.674	-2.006	1.00	0.57
ATOM 1605	CG2 THR 1 719	11.858	14.065	-0.477	1.00	0.57
ATOM 1606	N LYS 1 720	12.023	11.354	0.307	1.00	0.38
ATOM 1607	CA LYS 1 720	12.934	10.319	-0.099	1.00	0.38
ATOM 1608	C LYS 1 720	12.274	8.996	0.098	1.00	0.38
ATOM 1609	O LYS 1 720	12.531	8.055	-0.652	1.00	0.38
ATOM 1610	CB LYS 1 720	14.252	10.265	0.693	1.00	0.38
ATOM 1611	CG LYS 1 720	15.349	11.205	0.189	1.00	0.38
ATOM 1612	CD LYS 1 720	16.603	11.178	1.068	1.00	0.38
ATOM 1613	CE LYS 1 720	17.860	11.700	0.369	1.00	0.38
ATOM 1614	NZ LYS 1 720	19.019	11.637	1.288	1.00	0.38
ATOM 1615	N LEU 1 721	11.410	8.889	1.118	1.00	0.41
ATOM 1616	CA LEU 1 721	10.767	7.646	1.426	1.00	0.41
ATOM 1617	C LEU 1 721	9.983	7.235	0.221	1.00	0.41
ATOM 1618	O LEU 1 721	9.905	6.051	-0.104	1.00	0.41
ATOM 1619	CB LEU 1 721	9.819	7.794	2.641	1.00	0.41
ATOM 1620	CG LEU 1 721	9.144	6.513	3.195	1.00	0.41
ATOM 1621	CD1 LEU 1 721	8.249	6.867	4.393	1.00	0.41
ATOM 1622	CD2 LEU 1 721	8.357	5.719	2.139	1.00	0.41
ATOM 1623	N LEU 1 722	9.394	8.208	-0.496	1.00	0.46
ATOM 1624	CA LEU 1 722	8.576	7.876	-1.624	1.00	0.46
ATOM 1625	C LEU 1 722	9.408	7.127	-2.616	1.00	0.46

168/208

ATOM	1626	O	LEU 1 722	8.915	6.230	-3.299	1.00	0.46
ATOM	1627	CB	LEU 1 722	7.969	9.106	-2.310	1.00	0.46
ATOM	1628	CG	LEU 1 722	7.062	9.891	-1.348	1.00	0.46
ATOM	1629	CD1	LEU 1 722	5.991	8.978	-0.757	1.00	0.46
ATOM	1630	CD2	LEU 1 722	7.853	10.594	-0.247	1.00	0.46
ATOM	1631	N	ASP 1 723	10.702	7.472	-2.713	1.00	0.32
ATOM	1632	CA	ASP 1 723	11.577	6.833	-3.653	1.00	0.32
ATOM	1633	C	ASP 1 723	11.612	5.365	-3.353	1.00	0.32
ATOM	1634	O	ASP 1 723	11.535	4.538	-4.260	1.00	0.32
ATOM	1635	CB	ASP 1 723	13.016	7.366	-3.553	1.00	0.32
ATOM	1636	CG	ASP 1 723	13.820	6.816	-4.720	1.00	0.32
ATOM	1637	OD1	ASP 1 723	13.280	5.949	-5.460	1.00	0.32
ATOM	1638	OD2	ASP 1 723	14.986	7.261	-4.891	1.00	0.32
ATOM	1639	N	SER 1 724	11.725	4.993	-2.064	1.00	0.37
ATOM	1640	CA	SER 1 724	11.768	3.605	-1.698	1.00	0.37
ATOM	1641	C	SER 1 724	10.451	2.992	-2.035	1.00	0.37
ATOM	1642	O	SER 1 724	10.378	1.874	-2.545	1.00	0.37
ATOM	1643	CB	SER 1 724	11.996	3.386	-0.193	1.00	0.37
ATOM	1644	OG	SER 1 724	13.290	3.839	0.179	1.00	0.37
ATOM	1645	N	MET 1 725	9.361	3.729	-1.762	1.00	0.66
ATOM	1646	CA	MET 1 725	8.072	3.193	-2.052	1.00	0.66
ATOM	1647	C	MET 1 725	7.970	2.854	-3.501	1.00	0.66
ATOM	1648	O	MET 1 725	7.555	1.752	-3.852	1.00	0.66
ATOM	1649	CB	MET 1 725	6.932	4.153	-1.772	1.00	0.66
ATOM	1650	CG	MET 1 725	5.871	3.883	-2.820	1.00	0.66
ATOM	1651	SD	MET 1 725	4.224	3.695	-2.158	1.00	0.66
ATOM	1652	CE	MET 1 725	4.459	1.902	-2.141	1.00	0.66
ATOM	1653	N	HIS 1 726	8.371	3.782	-4.387	1.00	0.61
ATOM	1654	CA	HIS 1 726	8.237	3.502	-5.783	1.00	0.61
ATOM	1655	C	HIS 1 726	9.095	2.305	-6.065	1.00	0.61
ATOM	1656	O	HIS 1 726	8.780	1.475	-6.915	1.00	0.61
ATOM	1657	CB	HIS 1 726	8.711	4.639	-6.711	1.00	0.61
ATOM	1658	CG	HIS 1 726	10.055	4.399	-7.336	1.00	0.61
ATOM	1659	ND1	HIS 1 726	11.249	4.906	-6.875	1.00	0.61
ATOM	1660	CD2	HIS 1 726	10.368	3.665	-8.439	1.00	0.61
ATOM	1661	CE1	HIS 1 726	12.217	4.456	-7.713	1.00	0.61
ATOM	1662	NE2	HIS 1 726	11.731	3.696	-8.679	1.00	0.61
ATOM	1663	N	GLU 1 727	10.225	2.180	-5.350	1.00	0.31
ATOM	1664	CA	GLU 1 727	11.096	1.064	-5.583	1.00	0.31
ATOM	1665	C	GLU 1 727	10.346	-0.202	-5.309	1.00	0.31
ATOM	1666	O	GLU 1 727	10.375	-1.135	-6.109	1.00	0.31
ATOM	1667	CB	GLU 1 727	12.319	1.061	-4.647	1.00	0.31
ATOM	1668	CG	GLU 1 727	13.277	-0.115	-4.861	1.00	0.31
ATOM	1669	CD	GLU 1 727	14.217	0.223	-6.009	1.00	0.31
ATOM	1670	OE1	GLU 1 727	14.052	1.322	-6.600	1.00	0.31
ATOM	1671	OE2	GLU 1 727	15.116	-0.610	-6.307	1.00	0.31
ATOM	1672	N	VAL 1 728	9.625	-0.260	-4.173	1.00	0.24
ATOM	1673	CA	VAL 1 728	8.946	-1.466	-3.797	1.00	0.24
ATOM	1674	C	VAL 1 728	7.895	-1.812	-4.811	1.00	0.24
ATOM	1675	O	VAL 1 728	7.779	-2.966	-5.215	1.00	0.24
ATOM	1676	CB	VAL 1 728	8.270	-1.359	-2.460	1.00	0.24
ATOM	1677	CG1	VAL 1 728	7.544	-2.684	-2.179	1.00	0.24
ATOM	1678	CG2	VAL 1 728	9.328	-0.993	-1.403	1.00	0.24
ATOM	1679	N	VAL 1 729	7.106	-0.824	-5.277	1.00	0.27
ATOM	1680	CA	VAL 1 729	6.049	-1.153	-6.196	1.00	0.27
ATOM	1681	C	VAL 1 729	6.627	-1.732	-7.446	1.00	0.27
ATOM	1682	O	VAL 1 729	6.080	-2.685	-7.999	1.00	0.27
ATOM	1683	CB	VAL 1 729	5.187	0.011	-6.578	1.00	0.27
ATOM	1684	CG1	VAL 1 729	6.083	1.141	-7.070	1.00	0.27
ATOM	1685	CG2	VAL 1 729	4.225	-0.450	-7.682	1.00	0.27
ATOM	1686	N	GLU 1 730	7.755	-1.181	-7.930	1.00	0.20

169/208

ATOM 1687 CA GLU 1 730	8.331 -1.697 -9.137 1.00 0.20
ATOM 1688 C GLU 1 730	8.701 -3.128 -8.906 1.00 0.20
ATOM 1689 O GLU 1 730	8.432 -3.992 -9.739 1.00 0.20
ATOM 1690 CB GLU 1 730	9.622 -0.967 -9.548 1.00 0.20
ATOM 1691 CG GLU 1 730	9.411 0.480 -9.995 1.00 0.20
ATOM 1692 CD GLU 1 730	10.775 1.052 -10.361 1.00 0.20
ATOM 1693 OE1 GLU 1 730	11.795 0.364 -10.089 1.00 0.20
ATOM 1694 OE2 GLU 1 730	10.815 2.182 -10.918 1.00 0.20
ATOM 1695 N ASN 1 731	9.320 -3.425 -7.747 1.00 0.32
ATOM 1696 CA ASN 1 731	9.750 -4.770 -7.476 1.00 0.32
ATOM 1697 C ASN 1 731	8.540 -5.653 -7.428 1.00 0.32
ATOM 1698 O ASN 1 731	8.524 -6.750 -7.984 1.00 0.32
ATOM 1699 CB ASN 1 731	10.439 -4.911 -6.106 1.00 0.32
ATOM 1700 CG ASN 1 731	11.757 -4.150 -6.131 1.00 0.32
ATOM 1701 OD1 ASN 1 731	11.966 -3.220 -5.353 1.00 0.32
ATOM 1702 ND2 ASN 1 731	12.677 -4.561 -7.043 1.00 0.32
ATOM 1703 N LEU 1 732	7.485 -5.154 -6.767 1.00 0.58
ATOM 1704 CA LEU 1 732	6.243 -5.819 -6.490 1.00 0.58
ATOM 1705 C LEU 1 732	5.591 -6.183 -7.788 1.00 0.58
ATOM 1706 O LEU 1 732	5.074 -7.284 -7.968 1.00 0.58
ATOM 1707 CB LEU 1 732	5.328 -4.808 -5.758 1.00 0.58
ATOM 1708 CG LEU 1 732	3.972 -5.281 -5.199 1.00 0.58
ATOM 1709 CD1 LEU 1 732	3.073 -5.879 -6.288 1.00 0.58
ATOM 1710 CD2 LEU 1 732	4.136 -6.139 -3.935 1.00 0.58
ATOM 1711 N LEU 1 733	5.610 -5.243 -8.741 1.00 0.50
ATOM 1712 CA LEU 1 733	4.987 -5.442 -10.012 1.00 0.50
ATOM 1713 C LEU 1 733	5.675 -6.592 -10.665 1.00 0.50
ATOM 1714 O LEU 1 733	5.035 -7.455 -11.264 1.00 0.50
ATOM 1715 CB LEU 1 733	5.120 -4.169 -10.881 1.00 0.50
ATOM 1716 CG LEU 1 733	4.505 -4.206 -12.297 1.00 0.50
ATOM 1717 CD1 LEU 1 733	4.515 -2.802 -12.923 1.00 0.50
ATOM 1718 CD2 LEU 1 733	5.231 -5.199 -13.215 1.00 0.50
ATOM 1719 N ASN 1 734	7.011 -6.640 -10.542 1.00 0.49
ATOM 1720 CA ASN 1 734	7.777 -7.666 -11.173 1.00 0.49
ATOM 1721 C ASN 1 734	7.385 -8.993 -10.610 1.00 0.49
ATOM 1722 O ASN 1 734	7.142 -9.935 -11.364 1.00 0.49
ATOM 1723 CB ASN 1 734	9.285 -7.497 -10.929 1.00 0.49
ATOM 1724 CG ASN 1 734	9.726 -6.207 -11.606 1.00 0.49
ATOM 1725 OD1 ASN 1 734	10.835 -5.724 -11.385 1.00 0.49
ATOM 1726 ND2 ASN 1 734	8.829 -5.626 -12.446 1.00 0.49
ATOM 1727 N TYR 1 735	7.291 -9.120 -9.270 1.00 0.60
ATOM 1728 CA TYR 1 735	7.005 -10.439 -8.801 1.00 0.60
ATOM 1729 C TYR 1 735	5.599 -10.789 -9.177 1.00 0.60
ATOM 1730 O TYR 1 735	5.313 -11.930 -9.530 1.00 0.60
ATOM 1731 CB TYR 1 735	7.184 -10.691 -7.286 1.00 0.60
ATOM 1732 CG TYR 1 735	6.309 -11.797 -6.820 1.00 0.60
ATOM 1733 CD1 TYR 1 735	6.817 -13.073 -6.700 1.00 0.60
ATOM 1734 CD2 TYR 1 735	5.000 -11.570 -6.487 1.00 0.60
ATOM 1735 CE1 TYR 1 735	6.032 -14.115 -6.271 1.00 0.60
ATOM 1736 CE2 TYR 1 735	4.213 -12.610 -6.058 1.00 0.60
ATOM 1737 CZ TYR 1 735	4.720 -13.880 -5.945 1.00 0.60
ATOM 1738 OH TYR 1 735	3.896 -14.937 -5.502 1.00 0.60
ATOM 1739 N CYS 1 736	4.679 -9.807 -9.118 1.00 0.35
ATOM 1740 CA CYS 1 736	3.307 -10.089 -9.430 1.00 0.35
ATOM 1741 C CYS 1 736	3.190 -10.561 -10.845 1.00 0.35
ATOM 1742 O CYS 1 736	2.445 -11.495 -11.129 1.00 0.35
ATOM 1743 CB CYS 1 736	2.372 -8.880 -9.264 1.00 0.35
ATOM 1744 SG CYS 1 736	0.657 -9.282 -9.704 1.00 0.35
ATOM 1745 N PHE 1 737	3.916 -9.929 -11.781 1.00 0.23
ATOM 1746 CA PHE 1 737	3.843 -10.330 -13.159 1.00 0.23
ATOM 1747 C PHE 1 737	4.403 -11.702 -13.327 1.00 0.23

170/208

ATOM	1748	O	PHE 1737	3.948	-12.460	-14.182	1.00	0.23
ATOM	1749	CB	PHE 1737	4.580	-9.375	-14.112	1.00	0.23
ATOM	1750	CG	PHE 1737	3.649	-8.243	-14.374	1.00	0.23
ATOM	1751	CD1	PHE 1737	3.272	-7.390	-13.365	1.00	0.23
ATOM	1752	CD2	PHE 1737	3.162	-8.024	-15.642	1.00	0.23
ATOM	1753	CE1	PHE 1737	2.417	-6.343	-13.610	1.00	0.23
ATOM	1754	CE2	PHE 1737	2.307	-6.979	-15.897	1.00	0.23
ATOM	1755	CZ	PHE 1737	1.932	-6.135	-14.879	1.00	0.23
ATOM	1756	N	GLN 1738	5.406	-12.066	-12.510	1.00	0.51
ATOM	1757	CA	GLN 1738	6.023	-13.349	-12.668	1.00	0.51
ATOM	1758	C	GLN 1738	4.972	-14.401	-12.517	1.00	0.51
ATOM	1759	O	GLN 1738	4.969	-15.382	-13.259	1.00	0.51
ATOM	1760	CB	GLN 1738	7.117	-13.623	-11.624	1.00	0.51
ATOM	1761	CG	GLN 1738	7.780	-14.992	-11.789	1.00	0.51
ATOM	1762	CD	GLN 1738	8.835	-15.134	-10.704	1.00	0.51
ATOM	1763	OE1	GLN 1738	9.512	-16.157	-10.608	1.00	0.51
ATOM	1764	NE2	GLN 1738	8.986	-14.076	-9.863	1.00	0.51
ATOM	1765	N	THR 1739	4.048	-14.244	-11.550	1.00	0.90
ATOM	1766	CA	THR 1739	3.029	-15.247	-11.419	1.00	0.90
ATOM	1767	C	THR 1739	2.174	-15.225	-12.654	1.00	0.90
ATOM	1768	O	THR 1739	1.803	-16.279	-13.166	1.00	0.90
ATOM	1769	CB	THR 1739	2.142	-15.068	-10.217	1.00	0.90
ATOM	1770	OG1	THR 1739	1.347	-16.230	-10.027	1.00	0.90
ATOM	1771	CG2	THR 1739	1.232	-13.847	-10.419	1.00	0.90
ATOM	1772	N	PHE 1740	1.885	-14.006	-13.162	1.00	1.13
ATOM	1773	CA	PHE 1740	1.060	-13.667	-14.296	1.00	1.13
ATOM	1774	C	PHE 1740	-0.092	-14.595	-14.496	1.00	1.13
ATOM	1775	O	PHE 1740	0.046	-15.748	-14.904	1.00	1.13
ATOM	1776	CB	PHE 1740	1.801	-13.428	-15.632	1.00	1.13
ATOM	1777	CG	PHE 1740	2.485	-14.665	-16.094	1.00	1.13
ATOM	1778	CD1	PHE 1740	3.764	-14.948	-15.680	1.00	1.13
ATOM	1779	CD2	PHE 1740	1.856	-15.534	-16.954	1.00	1.13
ATOM	1780	CE1	PHE 1740	4.405	-16.086	-16.105	1.00	1.13
ATOM	1781	CE2	PHE 1740	2.491	-16.675	-17.384	1.00	1.13
ATOM	1782	CZ	PHE 1740	3.768	-16.953	-16.960	1.00	1.13
ATOM	1783	N	LEU 1741	-1.299	-14.062	-14.231	1.00	0.91
ATOM	1784	CA	LEU 1741	-2.516	-14.800	-14.363	1.00	0.91
ATOM	1785	C	LEU 1741	-2.585	-15.245	-15.795	1.00	0.91
ATOM	1786	O	LEU 1741	-1.798	-14.796	-16.627	1.00	0.91
ATOM	1787	CB	LEU 1741	-3.734	-13.946	-13.914	1.00	0.91
ATOM	1788	CG	LEU 1741	-5.116	-14.632	-13.813	1.00	0.91
ATOM	1789	CD1	LEU 1741	-6.063	-13.813	-12.921	1.00	0.91
ATOM	1790	CD2	LEU 1741	-5.774	-14.842	-15.181	1.00	0.91
ATOM	1791	N	ASP 1742	-3.497	-16.191	-16.097	1.00	0.71
ATOM	1792	CA	ASP 1742	-3.666	-16.809	-17.383	1.00	0.71
ATOM	1793	C	ASP 1742	-3.861	-15.793	-18.466	1.00	0.71
ATOM	1794	O	ASP 1742	-3.692	-14.590	-18.274	1.00	0.71
ATOM	1795	CB	ASP 1742	-4.868	-17.767	-17.437	1.00	0.71
ATOM	1796	CG	ASP 1742	-4.569	-18.945	-16.523	1.00	0.71
ATOM	1797	OD1	ASP 1742	-3.413	-19.028	-16.026	1.00	0.71
ATOM	1798	OD2	ASP 1742	-5.488	-19.779	-16.312	1.00	0.71
ATOM	1799	N	LYS 1743	-4.243	-16.293	-19.661	1.00	0.84
ATOM	1800	CA	LYS 1743	-4.406	-15.475	-20.827	1.00	0.84
ATOM	1801	C	LYS 1743	-5.329	-14.369	-20.453	1.00	0.84
ATOM	1802	O	LYS 1743	-5.007	-13.196	-20.640	1.00	0.84
ATOM	1803	CB	LYS 1743	-5.006	-16.263	-22.010	1.00	0.84
ATOM	1804	CG	LYS 1743	-5.190	-15.460	-23.300	1.00	0.84
ATOM	1805	CD	LYS 1743	-6.291	-14.398	-23.237	1.00	0.84
ATOM	1806	CE	LYS 1743	-7.656	-14.917	-23.697	1.00	0.84
ATOM	1807	NZ	LYS 1743	-8.094	-16.034	-22.830	1.00	0.84
ATOM	1808	N	THR 1744	-6.500	-14.709	-19.892	1.00	0.84

171/208

ATOM 1809	CA THR 1744	-7.332 -13.651 -19.420	1.00 0.84
ATOM 1810	C THR 1744	-6.812 -13.353 -18.055	1.00 0.84
ATOM 1811	O THR 1744	-7.419 -13.704 -17.045	1.00 0.84
ATOM 1812	CB THR 1744	-8.785 -14.025 -19.345	1.00 0.84
ATOM 1813	OG1 THR 1744	-8.976 -15.151 -18.500	1.00 0.84
ATOM 1814	CG2 THR 1744	-9.272 -14.343 -20.769	1.00 0.84
ATOM 1815	N MET 1745	-5.662 -12.654 -18.017	1.00 0.84
ATOM 1816	CA MET 1745	-4.952 -12.372 -16.808	1.00 0.84
ATOM 1817	C MET 1745	-5.849 -11.640 -15.886	1.00 0.84
ATOM 1818	O MET 1745	-5.684 -11.743 -14.673	1.00 0.84
ATOM 1819	CB MET 1745	-3.711 -11.490 -17.017	1.00 0.84
ATOM 1820	CG MET 1745	-2.968 -11.199 -15.713	1.00 0.84
ATOM 1821	SD MET 1745	-1.485 -10.163 -15.900	1.00 0.84
ATOM 1822	CE MET 1745	-1.092 -10.137 -14.128	1.00 0.84
ATOM 1823	N SER 1746	-6.793 -10.877 -16.467	1.00 1.05
ATOM 1824	CA SER 1746	-7.760 -10.055 -15.802	1.00 1.05
ATOM 1825	C SER 1746	-7.333 -8.683 -16.106	1.00 1.05
ATOM 1826	O SER 1746	-6.261 -8.265 -15.673	1.00 1.05
ATOM 1827	CB SER 1746	-7.886 -10.209 -14.269	1.00 1.05
ATOM 1828	OG SER 1746	-8.876 -9.333 -13.750	1.00 1.05
ATOM 1829	N ILE 1747	-8.164 -8.021 -16.932	1.00 1.19
ATOM 1830	CA ILE 1747	-8.108 -6.670 -17.393	1.00 1.19
ATOM 1831	C ILE 1747	-8.073 -5.783 -16.187	1.00 1.19
ATOM 1832	O ILE 1747	-9.044 -5.151 -15.774	1.00 1.19
ATOM 1833	CB ILE 1747	-9.231 -6.532 -18.420	1.00 1.19
ATOM 1834	CG1 ILE 1747	-8.658 -6.825 -19.821	1.00 1.19
ATOM 1835	CG2 ILE 1747	-10.165 -5.327 -18.267	1.00 1.19
ATOM 1836	CD1 ILE 1747	-8.097 -8.235 -19.995	1.00 1.19
ATOM 1837	N GLU 1748	-6.863 -5.764 -15.594	1.00 1.16
ATOM 1838	CA GLU 1748	-6.527 -5.086 -14.392	1.00 1.16
ATOM 1839	C GLU 1748	-6.244 -3.643 -14.601	1.00 1.16
ATOM 1840	O GLU 1748	-6.780 -2.817 -13.867	1.00 1.16
ATOM 1841	CB GLU 1748	-5.313 -5.690 -13.672	1.00 1.16
ATOM 1842	CG GLU 1748	-4.996 -4.930 -12.388	1.00 1.16
ATOM 1843	CD GLU 1748	-6.286 -4.866 -11.578	1.00 1.16
ATOM 1844	OE1 GLU 1748	-7.179 -5.725 -11.808	1.00 1.16
ATOM 1845	OE2 GLU 1748	-6.399 -3.946 -10.724	1.00 1.16
ATOM 1846	N PHE 1749	-5.380 -3.260 -15.565	1.00 1.07
ATOM 1847	CA PHE 1749	-5.167 -1.844 -15.542	1.00 1.07
ATOM 1848	C PHE 1749	-6.057 -0.830 -16.231	1.00 1.07
ATOM 1849	O PHE 1749	-6.666 -0.153 -15.426	1.00 1.07
ATOM 1850	CB PHE 1749	-3.708 -1.384 -15.525	1.00 1.07
ATOM 1851	CG PHE 1749	-3.490 -1.527 -14.058	1.00 1.07
ATOM 1852	CD1 PHE 1749	-4.079 -0.621 -13.203	1.00 1.07
ATOM 1853	CD2 PHE 1749	-2.740 -2.551 -13.532	1.00 1.07
ATOM 1854	CE1 PHE 1749	-3.924 -0.728 -11.843	1.00 1.07
ATOM 1855	CE2 PHE 1749	-2.580 -2.664 -12.172	1.00 1.07
ATOM 1856	CZ PHE 1749	-3.175 -1.757 -11.330	1.00 1.07
ATOM 1857	N PRO 1750	-6.247 -0.589 -17.529	1.00 0.90
ATOM 1858	CA PRO 1750	-7.221 0.431 -17.979	1.00 0.90
ATOM 1859	C PRO 1750	-8.771 0.442 -18.016	1.00 0.90
ATOM 1860	O PRO 1750	-9.291 1.473 -17.605	1.00 0.90
ATOM 1861	CB PRO 1750	-6.687 0.963 -19.305	1.00 0.90
ATOM 1862	CG PRO 1750	-5.169 0.827 -19.170	1.00 0.90
ATOM 1863	CD PRO 1750	-4.983 -0.372 -18.237	1.00 0.90
ATOM 1864	N GLU 1751	-9.539 -0.588 -18.489	1.00 0.84
ATOM 1865	CA GLU 1751	-11.014 -0.740 -18.539	1.00 0.84
ATOM 1866	C GLU 1751	-11.479 -0.956 -17.136	1.00 0.84
ATOM 1867	O GLU 1751	-12.611 -0.771 -16.702	1.00 0.84
ATOM 1868	CB GLU 1751	-11.508 -2.071 -19.129	1.00 0.84
ATOM 1869	CG GLU 1751	-11.246 -2.389 -20.592	1.00 0.84

172/208

ATOM	1870	CD	GLU	1751	-11.804	-3.799	-20.762	1.00	0.84
ATOM	1871	OE1	GLU	1751	-12.632	-4.206	-19.902	1.00	0.84
ATOM	1872	OE2	GLU	1751	-11.407	-4.491	-21.736	1.00	0.84
ATOM	1873	N	MET	1752	-10.435	-1.330	-16.468	1.00	1.00
ATOM	1874	CA	MET	1752	-9.749	-1.826	-15.370	1.00	1.00
ATOM	1875	C	MET	1752	-9.587	-0.479	-14.739	1.00	1.00
ATOM	1876	O	MET	1752	-9.038	0.421	-15.327	1.00	1.00
ATOM	1877	CB	MET	1752	-8.464	-2.412	-15.976	1.00	1.00
ATOM	1878	CG	MET	1752	-8.681	-2.977	-17.397	1.00	1.00
ATOM	1879	SD	MET	1752	-7.488	-3.879	-18.478	1.00	1.00
ATOM	1880	CE	MET	1752	-5.812	-3.234	-18.336	1.00	1.00
ATOM	1881	N	LEU	1753	-10.177	-0.119	-13.608	1.00	0.82
ATOM	1882	CA	LEU	1753	-10.723	1.132	-13.156	1.00	0.82
ATOM	1883	C	LEU	1753	-11.151	2.199	-14.132	1.00	0.82
ATOM	1884	O	LEU	1753	-11.750	3.146	-13.637	1.00	0.82
ATOM	1885	CB	LEU	1753	-9.733	1.821	-12.206	1.00	0.82
ATOM	1886	CG	LEU	1753	-9.134	0.865	-11.154	1.00	0.82
ATOM	1887	CD1	LEU	1753	-8.168	1.601	-10.215	1.00	0.82
ATOM	1888	CD2	LEU	1753	-10.213	0.066	-10.416	1.00	0.82
ATOM	1889	N	ALA	1754	-10.833	2.252	-15.434	1.00	0.46
ATOM	1890	CA	ALA	1754	-11.599	3.228	-16.176	1.00	0.46
ATOM	1891	C	ALA	1754	-13.059	2.905	-15.999	1.00	0.46
ATOM	1892	O	ALA	1754	-13.882	3.799	-15.806	1.00	0.46
ATOM	1893	CB	ALA	1754	-11.365	3.231	-17.693	1.00	0.46
ATOM	1894	N	GLU	1755	-13.440	1.617	-16.045	1.00	0.40
ATOM	1895	CA	GLU	1755	-14.834	1.335	-15.868	1.00	0.40
ATOM	1896	C	GLU	1755	-15.213	1.617	-14.439	1.00	0.40
ATOM	1897	O	GLU	1755	-16.289	2.147	-14.167	1.00	0.40
ATOM	1898	CB	GLU	1755	-15.219	-0.113	-16.213	1.00	0.40
ATOM	1899	CG	GLU	1755	-16.662	-0.249	-16.703	1.00	0.40
ATOM	1900	CD	GLU	1755	-16.704	0.257	-18.144	1.00	0.40
ATOM	1901	OE1	GLU	1755	-15.627	0.649	-18.670	1.00	0.40
ATOM	1902	OE2	GLU	1755	-17.815	0.259	-18.738	1.00	0.40
ATOM	1903	N	ILE	1756	-14.344	1.276	-13.465	1.00	0.54
ATOM	1904	CA	ILE	1756	-14.767	1.507	-12.107	1.00	0.54
ATOM	1905	C	ILE	1756	-14.871	2.980	-11.844	1.00	0.54
ATOM	1906	O	ILE	1756	-15.787	3.444	-11.166	1.00	0.54
ATOM	1907	CB	ILE	1756	-13.882	0.897	-11.056	1.00	0.54
ATOM	1908	CG1	ILE	1756	-14.628	0.842	-9.715	1.00	0.54
ATOM	1909	CG2	ILE	1756	-12.589	1.712	-10.964	1.00	0.54
ATOM	1910	CD1	ILE	1756	-13.948	-0.046	-8.675	1.00	0.54
ATOM	1911	N	ILE	1757	-13.918	3.756	-12.381	1.00	0.68
ATOM	1912	CA	ILE	1757	-13.860	5.171	-12.178	1.00	0.68
ATOM	1913	C	ILE	1757	-15.065	5.770	-12.829	1.00	0.68
ATOM	1914	O	ILE	1757	-15.686	6.676	-12.277	1.00	0.68
ATOM	1915	CB	ILE	1757	-12.586	5.766	-12.730	1.00	0.68
ATOM	1916	CG1	ILE	1757	-12.330	7.179	-12.179	1.00	0.68
ATOM	1917	CG2	ILE	1757	-12.629	5.683	-14.261	1.00	0.68
ATOM	1918	CD1	ILE	1757	-13.415	8.191	-12.530	1.00	0.68
ATOM	1919	N	THR	1758	-15.440	5.275	-14.024	1.00	0.66
ATOM	1920	CA	THR	1758	-16.587	5.825	-14.688	1.00	0.66
ATOM	1921	C	THR	1758	-17.817	5.482	-13.909	1.00	0.66
ATOM	1922	O	THR	1758	-18.720	6.305	-13.764	1.00	0.66
ATOM	1923	CB	THR	1758	-16.759	5.334	-16.101	1.00	0.66
ATOM	1924	OG1	THR	1758	-17.730	6.122	-16.773	1.00	0.66
ATOM	1925	CG2	THR	1758	-17.208	3.866	-16.084	1.00	0.66
ATOM	1926	N	ASN	1759	-17.878	4.251	-13.365	1.00	0.59
ATOM	1927	CA	ASN	1759	-19.051	3.827	-12.658	1.00	0.59
ATOM	1928	C	ASN	1759	-19.270	4.756	-11.512	1.00	0.59
ATOM	1929	O	ASN	1759	-20.380	5.246	-11.304	1.00	0.59
ATOM	1930	CB	ASN	1759	-18.912	2.404	-12.085	1.00	0.59

173/208

ATOM	1931	CG ASN 1 759	-20.216	2.021	-11.396	1.00	0.59
ATOM	1932	OD1 ASN 1 759	-20.634	2.642	-10.421	1.00	0.59
ATOM	1933	ND2 ASN 1 759	-20.885	0.959	-11.921	1.00	0.59
ATOM	1934	N GLN 1 760	-18.207	5.047	-10.745	1.00	0.63
ATOM	1935	CA GLN 1 760	-18.377	5.911	-9.617	1.00	0.63
ATOM	1936	C GLN 1 760	-18.731	7.261	-10.147	1.00	0.63
ATOM	1937	O GLN 1 760	-18.410	7.597	-11.286	1.00	0.63
ATOM	1938	CB GLN 1 760	-17.108	6.042	-8.759	1.00	0.63
ATOM	1939	CG GLN 1 760	-17.262	6.958	-7.545	1.00	0.63
ATOM	1940	CD GLN 1 760	-15.928	6.970	-6.815	1.00	0.63
ATOM	1941	OE1 GLN 1 760	-15.008	6.239	-7.179	1.00	0.63
ATOM	1942	NE2 GLN 1 760	-15.814	7.819	-5.758	1.00	0.63
ATOM	1943	N ILE 1 761	-19.443	8.061	-9.333	1.00	0.75
ATOM	1944	CA ILE 1 761	-19.806	9.378	-9.765	1.00	0.75
ATOM	1945	C ILE 1 761	-18.957	10.329	-8.920	1.00	0.75
ATOM	1946	O ILE 1 761	-18.295	9.822	-7.976	1.00	0.75
ATOM	1947	CB ILE 1 761	-21.261	9.689	-9.526	1.00	0.75
ATOM	1948	CG1 ILE 1 761	-22.144	8.673	-10.271	1.00	0.75
ATOM	1949	CG2 ILE 1 761	-21.544	11.138	-9.954	1.00	0.75
ATOM	1950	CD1 ILE 1 761	-23.618	8.746	-9.878	1.00	0.75
ATOM	1951	OXT ILE 1 761	-18.946	11.557	-9.202	1.00	99.99
TER	1952	ILE 1 761					
HETATM	1953	C01 UNK 1	-2.020	-7.470	-3.975	1.00	-0.03
HETATM	1954	C08 UNK 1	-2.604	-8.499	-4.716	1.00	0.00
HETATM	1955	C07 UNK 1	-3.588	-8.239	-5.676	1.00	0.00
HETATM	1956	C04 UNK 1	-4.044	-6.938	-5.927	1.00	0.15
HETATM	1957	C03 UNK 1	-3.449	-5.887	-5.194	1.00	0.00
HETATM	1958	C02 UNK 1	-2.450	-6.150	-4.229	1.00	0.00
HETATM	1959	N05 UNK 1	-5.088	-6.741	-6.891	1.00	-0.69
HETATM	1960	C06 UNK 1	-5.500	-7.809	-7.786	1.00	0.27
HETATM	1961	C09 UNK 1	-5.841	-5.513	-7.030	1.00	0.27
HETATM	1962	C19 C 2	2.863	-9.728	-3.299	1.00	0.02
HETATM	1963	C22 C 2	3.237	-10.282	-2.296	1.00	-0.39
HETATM	1964	C22 C 2	3.714	-10.953	-1.093	1.00	0.30
HETATM	1965	H100C 2	2.874	-11.106	-0.400	1.00	0.00
HETATM	1966	H101C 2	4.482	-10.332	-0.607	1.00	0.00
HETATM	1967	H102C 2	4.148	-11.927	-1.363	1.00	0.00
HETATM	1968	C01 UNK 3	-2.100	-6.783	-0.557	1.00	0.03
HETATM	1969	C02 UNK 3	-0.922	-6.070	-1.201	1.00	-0.03
HETATM	1970	C17 UNK 3	-0.435	-4.794	-0.622	1.00	-0.03
HETATM	1971	C16 UNK 3	0.740	-4.085	-1.251	1.00	0.03
HETATM	1972	C15 UNK 3	1.664	-5.067	-1.960	1.00	0.00
HETATM	1973	C14 UNK 3	0.923	-5.996	-2.938	1.00	0.14
HETATM	1974	C03 UNK 3	-0.344	-6.602	-2.292	1.00	-0.27
HETATM	1975	C04 UNK 3	-0.997	-7.843	-2.908	1.00	0.17
HETATM	1976	C05 UNK 3	0.077	-8.825	-3.425	1.00	0.00
HETATM	1977	C06 UNK 3	1.195	-8.166	-4.241	1.00	0.00
HETATM	1978	C07 UNK 3	0.631	-7.623	-5.568	1.00	0.00
HETATM	1979	C08 UNK 3	2.441	-9.040	-4.505	1.00	0.31
HETATM	1980	O09 UNK 3	2.272	-9.992	-5.534	1.00	-0.55
HETATM	1981	H10 UNK 3	1.590	-10.610	-5.262	1.00	0.31
HETATM	1982	C11 UNK 3	3.536	-8.012	-4.833	1.00	0.00
HETATM	1983	C12 UNK 3	3.149	-6.736	-4.082	1.00	0.00
HETATM	1984	C13 UNK 3	1.875	-7.132	-3.336	1.00	0.00
HETATM	1985	C18 UNK 3	-1.069	-4.259	0.508	1.00	0.00
HETATM	1986	C19 UNK 3	-2.258	-4.896	1.089	1.00	0.40
HETATM	1987	C21 UNK 3	-3.030	-5.873	0.233	1.00	0.05
HETATM	1988	O20 UNK 3	-2.621	-4.644	2.227	1.00	-0.45
CONECT	1953	1954 1958 1975					
CONECT	1954	1953 1955					
CONECT	1955	1954 1956					

174/208

CONNECT 1956 1955 1957 1959  
CONNECT 1957 1956 1958  
CONNECT 1958 1953 1957  
CONNECT 1959 1956 1960 1961  
CONNECT 1960 1959  
CONNECT 1961 1959  
CONNECT 1962 1963 1979  
CONNECT 1963 1962 1964  
CONNECT 1964 1963 1965 1966 1967  
CONNECT 1965 1964  
CONNECT 1966 1964  
CONNECT 1967 1964  
CONNECT 1968 1969 1987  
CONNECT 1969 1968 1970 1974  
CONNECT 1970 1969 1971 1985  
CONNECT 1971 1970 1972  
CONNECT 1972 1971 1973  
CONNECT 1973 1972 1974 1984  
CONNECT 1974 1969 1973 1975  
CONNECT 1975 1953 1974 1976  
CONNECT 1976 1975 1977  
CONNECT 1977 1976 1978 1979 1984  
CONNECT 1978 1977  
CONNECT 1979 1962 1977 1980 1982  
CONNECT 1980 1979 1981  
CONNECT 1981 1980  
CONNECT 1982 1979 1983  
CONNECT 1983 1982 1984  
CONNECT 1984 1973 1977 1983  
CONNECT 1985 1970 1986  
CONNECT 1986 1985 1987 1988  
CONNECT 1987 1968 1986  
CONNECT 1988 1986  
MASTER 0 0 0 0 0 0 0 0 0 1987 1 36 19  
END



175/208

HEADER PROTEIN 28-FEB-100  
COMPND GR\_TR\_V1  
AUTHOR GENERATED BY SYBYL, A PRODUCT OF TRIPOS, INC.  
SEQRES 1 1 240 PRO ALA THR LEU PRO GLN LEU THR PRO THR LEU VAL SER  
SEQRES 2 1 240 LEU LEU GLU VAL ILE GLU PRO GLU VAL LEU TYR ALA GLY  
SEQRES 3 1 240 TYR ASP SER SER VAL PRO ASP SER THR TRP ARG ILE MET  
SEQRES 4 1 240 THR THR LEU ASN MET LEU GLY GLY ARG GLN VAL ILE ALA  
SEQRES 5 1 240 ALA VAL LYS TRP ALA LYS ALA ILE PRO GLY PHE ARG ASN  
SEQRES 6 1 240 LEU HIS LEU ASP ASP GLN MET THR LEU LEU GLN TYR SER  
SEQRES 7 1 240 TRP MET PHE LEU MET ALA PHE ALA LEU GLY TRP ARG SER  
SEQRES 8 1 240 TYR ARG GLN SER SER ALA ASN LEU LEU CYS PHE ALA PRO  
SEQRES 9 1 240 ASP LEU ILE ILE ASN GLU GLN ARG MET THR LEU PRO CYS  
SEQRES 10 1 240 MET TYR ASP GLN CYS LYS HIS MET LEU TYR VAL SER SER  
SEQRES 11 1 240 GLU LEU HIS ARG LEU GLN VAL SER TYR GLU GLU TYR LEU  
SEQRES 12 1 240 CYS MET LYS THR LEU LEU LEU LEU SER SER VAL PRO LYS  
SEQRES 13 1 240 ASP GLY LEU LYS SER GLN GLU LEU PHE ASP GLU ILE ARG  
SEQRES 14 1 240 MET THR TYR ILE LYS GLU LEU GLY LYS ALA ILE VAL LYS  
SEQRES 15 1 240 ARG GLU GLY ASN SER SER GLN ASN TRP GLN ARG PHE TYR  
SEQRES 16 1 240 GLN LEU THR LYS LEU LEU ASP SER MET HIS GLU VAL VAL  
SEQRES 17 1 240 GLU ASN LEU LEU ASN TYR CYS PHE GLN THR PHE LEU ASP  
SEQRES 18 1 240 LYS THR MET SER ILE GLU PHE PRO GLU MET LEU ALA GLU  
SEQRES 19 1 240 ILE ILE THR ASN GLN ILE  
ATOM 1 N PRO 1 522 -0.627 29.241 5.806 1.00 5.52  
ATOM 2 CA PRO 1 522 -1.732 29.968 5.121 1.00 5.52  
ATOM 3 C PRO 1 522 -3.005 29.229 5.366 1.00 5.52  
ATOM 4 O PRO 1 522 -2.966 28.016 5.546 1.00 5.52  
ATOM 5 CB PRO 1 522 -1.324 30.082 3.655 1.00 5.52  
ATOM 6 CG PRO 1 522 0.209 30.020 3.670 1.00 5.52  
ATOM 7 CD PRO 1 522 0.557 29.143 4.882 1.00 5.52  
ATOM 8 N ALA 1 523 -4.144 29.942 5.367 1.00 0.96  
ATOM 9 CA ALA 1 523 -5.430 29.392 5.693 1.00 0.96  
ATOM 10 C ALA 1 523 -5.899 28.334 4.745 1.00 0.96  
ATOM 11 O ALA 1 523 -6.411 27.298 5.168 1.00 0.96  
ATOM 12 CB ALA 1 523 -6.527 30.469 5.724 1.00 0.96  
ATOM 13 N THR 1 524 -5.708 28.546 3.432 1.00 5.12  
ATOM 14 CA THR 1 524 -6.270 27.645 2.469 1.00 5.12  
ATOM 15 C THR 1 524 -5.769 26.255 2.661 1.00 5.12  
ATOM 16 O THR 1 524 -6.508 25.289 2.476 1.00 5.12  
ATOM 17 CB THR 1 524 -5.970 28.028 1.048 1.00 5.12  
ATOM 18 OG1 THR 1 524 -6.738 27.228 0.161 1.00 5.12  
ATOM 19 CG2 THR 1 524 -4.469 27.825 0.775 1.00 5.12  
ATOM 20 N LEU 1 525 -4.495 26.116 3.050 1.00 4.05  
ATOM 21 CA LEU 1 525 -3.904 24.817 3.148 1.00 4.05  
ATOM 22 C LEU 1 525 -4.619 23.998 4.180 1.00 4.05  
ATOM 23 O LEU 1 525 -4.846 22.807 3.975 1.00 4.05  
ATOM 24 CB LEU 1 525 -2.406 24.884 3.473 1.00 4.05  
ATOM 25 CG LEU 1 525 -1.624 25.796 2.496 1.00 4.05  
ATOM 26 CD1 LEU 1 525 -1.808 25.375 1.030 1.00 4.05  
ATOM 27 CD2 LEU 1 525 -1.952 27.279 2.714 1.00 4.05  
ATOM 28 N PRO 1 526 -4.986 24.583 5.282 1.00 2.45  
ATOM 29 CA PRO 1 526 -5.729 23.833 6.245 1.00 2.45  
ATOM 30 C PRO 1 526 -7.071 23.501 5.695 1.00 2.45  
ATOM 31 O PRO 1 526 -7.745 22.642 6.253 1.00 2.45  
ATOM 32 CB PRO 1 526 -5.728 24.660 7.535 1.00 2.45  
ATOM 33 CG PRO 1 526 -4.888 25.909 7.201 1.00 2.45  
ATOM 34 CD PRO 1 526 -4.087 25.487 5.960 1.00 2.45  
ATOM 35 N GLN 1 527 -7.532 24.178 4.638 1.00 6.73  
ATOM 36 CA GLN 1 527 -8.784 23.731 4.111 1.00 6.73  
ATOM 37 C GLN 1 527 -8.494 22.376 3.553 1.00 6.73  
ATOM 38 O GLN 1 527 -9.217 21.409 3.789 1.00 6.73  
ATOM 39 CB GLN 1 527 -9.294 24.611 2.957 1.00 6.73

SUBSTITUTE SHEET (RULE 26)

176/208

ATOM	40	CG	GLN	1 527	-10.650	24.176	2.394	1.00	6.73
ATOM	41	CD	GLN	1 527	-11.731	24.634	3.365	1.00	6.73
ATOM	42	OE1	GLN	1 527	-12.924	24.477	3.113	1.00	6.73
ATOM	43	NE2	GLN	1 527	-11.299	25.225	4.511	1.00	6.73
ATOM	44	N	LEU	1 528	-7.375	22.285	2.811	1.00	1.25
ATOM	45	CA	LEU	1 528	-6.989	21.077	2.149	1.00	1.25
ATOM	46	C	LEU	1 528	-6.605	19.985	3.099	1.00	1.25
ATOM	47	O	LEU	1 528	-6.949	18.826	2.873	1.00	1.25
ATOM	48	CB	LEU	1 528	-5.827	21.278	1.167	1.00	1.25
ATOM	49	CG	LEU	1 528	-5.404	19.980	0.459	1.00	1.25
ATOM	50	CD1	LEU	1 528	-6.589	19.354	-0.296	1.00	1.25
ATOM	51	CD2	LEU	1 528	-4.197	20.216	-0.460	1.00	1.25
ATOM	52	N	THR	1 529	-5.883	20.309	4.187	1.00	5.96
ATOM	53	CA	THR	1 529	-5.449	19.243	5.042	1.00	5.96
ATOM	54	C	THR	1 529	-6.567	18.468	5.692	1.00	5.96
ATOM	55	O	THR	1 529	-6.499	17.241	5.674	1.00	5.96
ATOM	56	CB	THR	1 529	-4.353	19.648	6.007	1.00	5.96
ATOM	57	OG1	THR	1 529	-4.145	18.629	6.974	1.00	5.96
ATOM	58	CG2	THR	1 529	-4.595	21.030	6.638	1.00	5.96
ATOM	59	N	PRO	1 530	-7.594	19.043	6.263	1.00	5.19
ATOM	60	CA	PRO	1 530	-8.631	18.171	6.732	1.00	5.19
ATOM	61	C	PRO	1 530	-9.396	17.473	5.656	1.00	5.19
ATOM	62	O	PRO	1 530	-9.961	16.419	5.940	1.00	5.19
ATOM	63	CB	PRO	1 530	-9.480	18.989	7.697	1.00	5.19
ATOM	64	CG	PRO	1 530	-8.446	19.924	8.336	1.00	5.19
ATOM	65	CD	PRO	1 530	-7.367	20.075	7.254	1.00	5.19
ATOM	66	N	THR	1 531	-9.457	18.027	4.431	1.00	0.64
ATOM	67	CA	THR	1 531	-10.190	17.352	3.401	1.00	0.64
ATOM	68	C	THR	1 531	-9.495	16.061	3.114	1.00	0.64
ATOM	69	O	THR	1 531	-10.110	14.995	3.091	1.00	0.64
ATOM	70	CB	THR	1 531	-10.231	18.143	2.127	1.00	0.64
ATOM	71	OG1	THR	1 531	-10.823	19.412	2.362	1.00	0.64
ATOM	72	CG2	THR	1 531	-11.054	17.364	1.088	1.00	0.64
ATOM	73	N	LEU	1 532	-8.165	16.133	2.924	1.00	6.54
ATOM	74	CA	LEU	1 532	-7.401	14.967	2.608	1.00	6.54
ATOM	75	C	LEU	1 532	-7.451	14.010	3.750	1.00	6.54
ATOM	76	O	LEU	1 532	-7.628	12.816	3.537	1.00	6.54
ATOM	77	CB	LEU	1 532	-5.939	15.288	2.227	1.00	6.54
ATOM	78	CG	LEU	1 532	-5.114	16.074	3.268	1.00	6.54
ATOM	79	CD1	LEU	1 532	-4.690	15.205	4.462	1.00	6.54
ATOM	80	CD2	LEU	1 532	-3.922	16.777	2.601	1.00	6.54
ATOM	81	N	VAL	1 533	-7.357	14.496	4.997	1.00	0.78
ATOM	82	CA	VAL	1 533	-7.312	13.615	6.132	1.00	0.78
ATOM	83	C	VAL	1 533	-8.569	12.811	6.247	1.00	0.78
ATOM	84	O	VAL	1 533	-8.524	11.602	6.475	1.00	0.78
ATOM	85	CB	VAL	1 533	-7.153	14.365	7.416	1.00	0.78
ATOM	86	CG1	VAL	1 533	-7.253	13.368	8.578	1.00	0.78
ATOM	87	CG2	VAL	1 533	-5.825	15.139	7.368	1.00	0.78
ATOM	88	N	SER	1 534	-9.730	13.465	6.071	1.00	2.96
ATOM	89	CA	SER	1 534	-10.989	12.790	6.208	1.00	2.96
ATOM	90	C	SER	1 534	-11.018	11.730	5.164	1.00	2.96
ATOM	91	O	SER	1 534	-11.546	10.637	5.366	1.00	2.96
ATOM	92	CB	SER	1 534	-12.192	13.718	5.971	1.00	2.96
ATOM	93	OG	SER	1 534	-13.404	12.993	6.116	1.00	2.96
ATOM	94	N	LEU	1 535	-10.418	12.049	4.013	1.00	7.50
ATOM	95	CA	LEU	1 535	-10.349	11.153	2.910	1.00	7.50
ATOM	96	C	LEU	1 535	-9.730	9.848	3.293	1.00	7.50
ATOM	97	O	LEU	1 535	-10.320	8.802	3.027	1.00	7.50
ATOM	98	CB	LEU	1 535	-9.471	11.746	1.819	1.00	7.50
ATOM	99	CG	LEU	1 535	-9.060	10.667	0.844	1.00	7.50
ATOM	100	CD1	LEU	1 535	-10.323	9.945	0.376	1.00	7.50

177 / 208

ATOM	101	CD2 LEU 1 535	-8.144	11.236	-0.247	1.00	7.50
ATOM	102	N LEU 1 536	-8.535	9.854	3.922	1.00	5.15
ATOM	103	CA LEU 1 536	-7.959	8.579	4.258	1.00	5.15
ATOM	104	C LEU 1 536	-8.747	7.902	5.310	1.00	5.15
ATOM	105	O LEU 1 536	-8.938	6.691	5.244	1.00	5.15
ATOM	106	CB LEU 1 536	-6.518	8.550	4.791	1.00	5.15
ATOM	107	CG LEU 1 536	-5.926	7.169	5.143	1.00	5.15
ATOM	108	CD1 LEU 1 536	-6.389	6.648	6.514	1.00	5.15
ATOM	109	CD2 LEU 1 536	-6.182	6.173	4.004	1.00	5.15
ATOM	110	N GLU 1 537	-9.215	8.674	6.306	1.00	3.32
ATOM	111	CA GLU 1 537	-9.876	8.087	7.433	1.00	3.32
ATOM	112	C GLU 1 537	-11.004	7.253	6.936	1.00	3.32
ATOM	113	O GLU 1 537	-11.180	6.113	7.366	1.00	3.32
ATOM	114	CB GLU 1 537	-10.491	9.139	8.375	1.00	3.32
ATOM	115	CG GLU 1 537	-9.466	9.988	9.130	1.00	3.32
ATOM	116	CD GLU 1 537	-8.937	9.165	10.295	1.00	3.32
ATOM	117	OE1 GLU 1 537	-8.074	9.692	11.047	1.00	3.32
ATOM	118	OE2 GLU 1 537	-9.391	8.000	10.453	1.00	3.32
ATOM	119	N VAL 1 538	-11.787	7.791	5.989	1.00	4.21
ATOM	120	CA VAL 1 538	-12.906	7.043	5.514	1.00	4.21
ATOM	121	C VAL 1 538	-12.485	5.790	4.802	1.00	4.21
ATOM	122	O VAL 1 538	-13.042	4.726	5.058	1.00	4.21
ATOM	123	CB VAL 1 538	-13.781	7.832	4.581	1.00	4.21
ATOM	124	CG1 VAL 1 538	-14.337	9.043	5.348	1.00	4.21
ATOM	125	CG2 VAL 1 538	-12.978	8.204	3.325	1.00	4.21
ATOM	126	N ILE 1 539	-11.500	5.860	3.880	1.00	8.15
ATOM	127	CA ILE 1 539	-11.192	4.652	3.161	1.00	8.15
ATOM	128	C ILE 1 539	-10.371	3.670	3.930	1.00	8.15
ATOM	129	O ILE 1 539	-10.401	2.484	3.614	1.00	8.15
ATOM	130	CB ILE 1 539	-10.538	4.768	1.805	1.00	8.15
ATOM	131	CG1 ILE 1 539	-9.065	5.184	1.864	1.00	8.15
ATOM	132	CG2 ILE 1 539	-11.410	5.716	0.966	1.00	8.15
ATOM	133	CD1 ILE 1 539	-8.851	6.612	2.298	1.00	8.15
ATOM	134	N GLU 1 540	-9.571	4.137	4.909	1.00	4.12
ATOM	135	CA GLU 1 540	-8.724	3.247	5.654	1.00	4.12
ATOM	136	C GLU 1 540	-9.574	2.205	6.301	1.00	4.12
ATOM	137	O GLU 1 540	-10.537	2.507	7.004	1.00	4.12
ATOM	138	CB GLU 1 540	-7.933	3.953	6.769	1.00	4.12
ATOM	139	CG GLU 1 540	-7.018	3.017	7.560	1.00	4.12
ATOM	140	CD GLU 1 540	-6.307	3.845	8.622	1.00	4.12
ATOM	141	OE1 GLU 1 540	-5.440	3.273	9.335	1.00	4.12
ATOM	142	OE2 GLU 1 540	-6.626	5.058	8.737	1.00	4.12
ATOM	143	N PRO 1 541	-9.231	0.969	6.072	1.00	5.53
ATOM	144	CA PRO 1 541	-10.006	-0.080	6.661	1.00	5.53
ATOM	145	C PRO 1 541	-9.704	-0.127	8.111	1.00	5.53
ATOM	146	O PRO 1 541	-8.615	0.310	8.476	1.00	5.53
ATOM	147	CB PRO 1 541	-9.637	-1.354	5.904	1.00	5.53
ATOM	148	CG PRO 1 541	-9.217	-0.837	4.517	1.00	5.53
ATOM	149	CD PRO 1 541	-8.676	0.577	4.786	1.00	5.53
ATOM	150	N GLU 1 542	-10.669	-0.632	8.912	1.00	6.38
ATOM	151	CA GLU 1 542	-10.594	-0.794	10.337	1.00	6.38
ATOM	152	C GLU 1 542	-9.653	0.163	10.975	1.00	6.38
ATOM	153	O GLU 1 542	-8.445	-0.062	10.977	1.00	6.38
ATOM	154	CB GLU 1 542	-10.213	-2.215	10.784	1.00	6.38
ATOM	155	CG GLU 1 542	-11.367	-3.220	10.712	1.00	6.38
ATOM	156	CD GLU 1 542	-11.704	-3.495	9.254	1.00	6.38
ATOM	157	OE1 GLU 1 542	-12.351	-2.620	8.618	1.00	6.38
ATOM	158	OE2 GLU 1 542	-11.328	-4.590	8.758	1.00	6.38
ATOM	159	N VAL 1 543	-10.188	1.285	11.490	1.00	2.42
ATOM	160	CA VAL 1 543	-9.342	2.211	12.175	1.00	2.42
ATOM	161	C VAL 1 543	-8.738	1.383	13.264	1.00	2.42

178/208

ATOM	162	O	VAL	1 543	-7.553	1.510	13.567	1.00	2.42
ATOM	163	CB	VAL	1 543	-10.100	3.338	12.810	1.00	2.42
ATOM	164	CG1	VAL	1 543	-9.104	4.218	13.584	1.00	2.42
ATOM	165	CG2	VAL	1 543	-10.870	4.089	11.711	1.00	2.42
ATOM	166	N	LEU	1 544	-9.546	0.467	13.843	1.00	7.00
ATOM	167	CA	LEU	1 544	-9.040	-0.416	14.851	1.00	7.00
ATOM	168	C	LEU	1 544	-7.965	-1.188	14.158	1.00	7.00
ATOM	169	O	LEU	1 544	-8.090	-1.557	12.992	1.00	7.00
ATOM	170	CB	LEU	1 544	-10.117	-1.354	15.443	1.00	7.00
ATOM	171	CG	LEU	1 544	-9.644	-2.308	16.564	1.00	7.00
ATOM	172	CD1	LEU	1 544	-10.842	-3.017	17.209	1.00	7.00
ATOM	173	CD2	LEU	1 544	-8.606	-3.330	16.075	1.00	7.00
ATOM	174	N	TYR	1 545	-6.872	-1.457	14.883	1.00	9.50
ATOM	175	CA	TYR	1 545	-5.668	-1.991	14.326	1.00	9.50
ATOM	176	C	TYR	1 545	-5.530	-3.441	14.662	1.00	9.50
ATOM	177	O	TYR	1 545	-6.141	-4.317	14.047	1.00	9.50
ATOM	178	CB	TYR	1 545	-4.490	-1.241	14.972	1.00	9.50
ATOM	179	CG	TYR	1 545	-3.181	-1.414	14.291	1.00	9.50
ATOM	180	CD1	TYR	1 545	-2.875	-0.615	13.212	1.00	9.50
ATOM	181	CD2	TYR	1 545	-2.157	-2.048	14.954	1.00	9.50
ATOM	182	CE1	TYR	1 545	-1.574	-0.459	12.796	1.00	9.50
ATOM	183	CE2	TYR	1 545	-0.854	-1.898	14.545	1.00	9.50
ATOM	184	CZ	TYR	1 545	-0.560	-1.084	13.481	1.00	9.50
ATOM	185	OH	TYR	1 545	0.787	-0.832	13.147	1.00	9.50
ATOM	186	N	ALA	1 546	-4.692	-3.708	15.676	1.00	1.35
ATOM	187	CA	ALA	1 546	-4.340	-5.025	16.109	1.00	1.35
ATOM	188	C	ALA	1 546	-5.523	-5.783	16.607	1.00	1.35
ATOM	189	O	ALA	1 546	-5.545	-7.007	16.515	1.00	1.35
ATOM	190	CB	ALA	1 546	-3.300	-5.025	17.242	1.00	1.35
ATOM	191	N	GLY	1 547	-6.535	-5.086	17.151	1.00	1.27
ATOM	192	CA	GLY	1 547	-7.639	-5.775	17.755	1.00	1.27
ATOM	193	C	GLY	1 547	-8.252	-6.802	16.851	1.00	1.27
ATOM	194	O	GLY	1 547	-8.407	-7.954	17.251	1.00	1.27
ATOM	195	N	TYR	1 548	-8.598	-6.437	15.601	1.00	2.17
ATOM	196	CA	TYR	1 548	-9.253	-7.419	14.782	1.00	2.17
ATOM	197	C	TYR	1 548	-8.395	-7.952	13.677	1.00	2.17
ATOM	198	O	TYR	1 548	-8.822	-7.969	12.525	1.00	2.17
ATOM	199	CB	TYR	1 548	-10.529	-6.897	14.101	1.00	2.17
ATOM	200	CG	TYR	1 548	-11.566	-6.699	15.150	1.00	2.17
ATOM	201	CD1	TYR	1 548	-11.629	-5.525	15.864	1.00	2.17
ATOM	202	CD2	TYR	1 548	-12.485	-7.689	15.406	1.00	2.17
ATOM	203	CE1	TYR	1 548	-12.607	-5.344	16.814	1.00	2.17
ATOM	204	CE2	TYR	1 548	-13.461	-7.513	16.357	1.00	2.17
ATOM	205	CZ	TYR	1 548	-13.525	-6.335	17.060	1.00	2.17
ATOM	206	OH	TYR	1 548	-14.517	-6.151	18.046	1.00	2.17
ATOM	207	N	ASP	1 549	-7.177	-8.436	13.981	1.00	5.55
ATOM	208	CA	ASP	1 549	-6.380	-8.969	12.912	1.00	5.55
ATOM	209	C	ASP	1 549	-6.134	-10.427	13.168	1.00	5.55
ATOM	210	O	ASP	1 549	-6.262	-10.894	14.297	1.00	5.55
ATOM	211	CB	ASP	1 549	-5.014	-8.281	12.761	1.00	5.55
ATOM	212	CG	ASP	1 549	-4.212	-8.527	14.029	1.00	5.55
ATOM	213	OD1	ASP	1 549	-2.972	-8.307	13.984	1.00	5.55
ATOM	214	OD2	ASP	1 549	-4.816	-8.944	15.053	1.00	5.55
ATOM	215	N	SER	1 550	-5.790	-11.196	12.113	1.00	0.80
ATOM	216	CA	SER	1 550	-5.537	-12.600	12.289	1.00	0.80
ATOM	217	C	SER	1 550	-4.246	-12.948	11.606	1.00	0.80
ATOM	218	O	SER	1 550	-3.812	-12.245	10.695	1.00	0.80
ATOM	219	CB	SER	1 550	-6.620	-13.499	11.672	1.00	0.80
ATOM	220	OG	SER	1 550	-6.619	-13.359	10.259	1.00	0.80
ATOM	221	N	SER	1 551	-3.594	-14.046	12.051	1.00	3.97
ATOM	222	CA	SER	1 551	-2.348	-14.482	11.474	1.00	3.97

179/208

ATOM	223	C	SER	1	551	-2.628	-15.435	10.351	1.00	3.97
ATOM	224	O	SER	1	551	-3.668	-16.089	10.330	1.00	3.97
ATOM	225	CB	SER	1	551	-1.416	-15.187	12.477	1.00	3.97
ATOM	226	OG	SER	1	551	-2.010	-16.390	12.944	1.00	3.97
ATOM	227	N	VAL	1	552	-1.703	-15.526	9.363	1.00	2.63
ATOM	228	CA	VAL	1	552	-1.933	-16.318	8.175	1.00	2.63
ATOM	229	C	VAL	1	552	-0.573	-16.748	7.601	1.00	2.63
ATOM	230	O	VAL	1	552	0.265	-15.862	7.505	1.00	2.63
ATOM	231	CB	VAL	1	552	-2.676	-15.415	7.202	1.00	2.63
ATOM	232	CG1	VAL	1	552	-2.855	-16.023	5.823	1.00	2.63
ATOM	233	CG2	VAL	1	552	-4.042	-15.059	7.811	1.00	2.63
ATOM	234	N	PRO	1	553	-0.231	-18.027	7.329	1.00	9.93
ATOM	235	CA	PRO	1	553	1.065	-18.358	6.679	1.00	9.93
ATOM	236	C	PRO	1	553	1.126	-18.968	5.236	1.00	9.93
ATOM	237	O	PRO	1	553	0.475	-19.998	5.072	1.00	9.93
ATOM	238	CB	PRO	1	553	1.784	-19.288	7.649	1.00	9.93
ATOM	239	CG	PRO	1	553	0.631	-20.005	8.368	1.00	9.93
ATOM	240	CD	PRO	1	553	-0.490	-18.956	8.420	1.00	9.93
ATOM	241	N	ASP	1	554	1.928	-18.474	4.211	1.00	7.69
ATOM	242	CA	ASP	1	554	2.026	-19.177	2.915	1.00	7.69
ATOM	243	C	ASP	1	554	2.850	-18.555	1.745	1.00	7.69
ATOM	244	O	ASP	1	554	3.467	-17.502	1.910	1.00	7.69
ATOM	245	CB	ASP	1	554	0.671	-19.618	2.359	1.00	7.69
ATOM	246	CG	ASP	1	554	0.992	-20.935	1.676	1.00	7.69
ATOM	247	OD1	ASP	1	554	2.167	-21.375	1.764	1.00	7.69
ATOM	248	OD2	ASP	1	554	0.069	-21.531	1.072	1.00	7.69
ATOM	249	N	SER	1	555	2.873	-19.195	0.516	1.00	5.28
ATOM	250	CA	SER	1	555	3.725	-18.879	-0.634	1.00	5.28
ATOM	251	C	SER	1	555	2.970	-18.889	-1.948	1.00	5.28
ATOM	252	O	SER	1	555	1.762	-19.104	-1.955	1.00	5.28
ATOM	253	CB	SER	1	555	4.897	-19.883	-0.739	1.00	5.28
ATOM	254	OG	SER	1	555	5.767	-19.577	-1.819	1.00	5.28
ATOM	255	N	THR	1	556	3.665	-18.594	-3.079	1.00	9.81
ATOM	256	CA	THR	1	556	3.098	-18.498	-4.399	1.00	9.81
ATOM	257	C	THR	1	556	2.078	-19.549	-4.606	1.00	9.81
ATOM	258	O	THR	1	556	2.322	-20.712	-4.296	1.00	9.81
ATOM	259	CB	THR	1	556	4.110	-18.631	-5.498	1.00	9.81
ATOM	260	OG1	THR	1	556	4.727	-19.910	-5.444	1.00	9.81
ATOM	261	CG2	THR	1	556	5.165	-17.525	-5.339	1.00	9.81
ATOM	262	N	TRP	1	557	0.895	-19.108	-5.085	1.00	5.43
ATOM	263	CA	TRP	1	557	-0.253	-19.917	-5.357	1.00	5.43
ATOM	264	C	TRP	1	557	-1.190	-19.773	-4.203	1.00	5.43
ATOM	265	O	TRP	1	557	-2.096	-18.941	-4.231	1.00	5.43
ATOM	266	CB	TRP	1	557	0.057	-21.409	-5.621	1.00	5.43
ATOM	267	CG	TRP	1	557	0.908	-21.586	-6.860	1.00	5.43
ATOM	268	CD1	TRP	1	557	1.247	-20.638	-7.782	1.00	5.43
ATOM	269	CD2	TRP	1	557	1.570	-22.798	-7.266	1.00	5.43
ATOM	270	NE1	TRP	1	557	2.062	-21.184	-8.742	1.00	5.43
ATOM	271	CE2	TRP	1	557	2.273	-22.511	-8.437	1.00	5.43
ATOM	272	CE3	TRP	1	557	1.595	-24.046	-6.710	1.00	5.43
ATOM	273	CZ2	TRP	1	557	3.012	-23.468	-9.072	1.00	5.43
ATOM	274	CZ3	TRP	1	557	2.341	-25.008	-7.354	1.00	5.43
ATOM	275	CH2	TRP	1	557	3.037	-24.726	-8.512	1.00	5.43
ATOM	276	N	ARG	1	558	-0.986	-20.580	-3.147	1.00	4.12
ATOM	277	CA	ARG	1	558	-1.870	-20.583	-2.018	1.00	4.12
ATOM	278	C	ARG	1	558	-1.869	-19.291	-1.243	1.00	4.12
ATOM	279	O	ARG	1	558	-2.939	-18.741	-0.987	1.00	4.12
ATOM	280	CB	ARG	1	558	-1.570	-21.770	-1.089	1.00	4.12
ATOM	281	CG	ARG	1	558	-2.483	-21.915	0.132	1.00	4.12
ATOM	282	CD	ARG	1	558	-2.129	-23.147	0.976	1.00	4.12
ATOM	283	NE	ARG	1	558	-2.927	-23.111	2.231	1.00	4.12

180/208

ATOM	284	CZ	ARG	1	558	-4.086	-23.824	2.321	1.00	4.12
ATOM	285	NH1	ARG	1	558	-4.518	-24.562	1.258	1.00	4.12
ATOM	286	NH2	ARG	1	558	-4.799	-23.816	3.484	1.00	4.12
ATOM	287	N	ILE	1	559	-0.695	-18.747	-0.843	1.00	7.58
ATOM	288	CA	ILE	1	559	-0.761	-17.491	-0.136	1.00	7.58
ATOM	289	C	ILE	1	559	-1.163	-16.455	-1.122	1.00	7.58
ATOM	290	O	ILE	1	559	-1.922	-15.554	-0.783	1.00	7.58
ATOM	291	CB	ILE	1	559	0.492	-17.071	0.590	1.00	7.58
ATOM	292	CG1	ILE	1	559	0.360	-15.803	1.440	1.00	7.58
ATOM	293	CG2	ILE	1	559	1.567	-16.870	-0.411	1.00	7.58
ATOM	294	CD1	ILE	1	559	-0.030	-14.472	0.828	1.00	7.58
ATOM	295	N	MET	1	560	-0.726	-16.591	-2.389	1.00	1.02
ATOM	296	CA	MET	1	560	-1.077	-15.624	-3.390	1.00	1.02
ATOM	297	C	MET	1	560	-2.568	-15.530	-3.413	1.00	1.02
ATOM	298	O	MET	1	560	-3.133	-14.446	-3.546	1.00	1.02
ATOM	299	CB	MET	1	560	-0.619	-16.020	-4.805	1.00	1.02
ATOM	300	CG	MET	1	560	-0.959	-14.967	-5.865	1.00	1.02
ATOM	301	SD	MET	1	560	-0.338	-15.332	-7.535	1.00	1.02
ATOM	302	CE	MET	1	560	-1.515	-16.668	-7.887	1.00	1.02
ATOM	303	N	THR	1	561	-3.245	-16.676	-3.233	1.00	0.75
ATOM	304	CA	THR	1	561	-4.675	-16.664	-3.213	1.00	0.75
ATOM	305	C	THR	1	561	-5.142	-15.836	-2.058	1.00	0.75
ATOM	306	O	THR	1	561	-6.070	-15.039	-2.189	1.00	0.75
ATOM	307	CB	THR	1	561	-5.280	-18.020	-3.010	1.00	0.75
ATOM	308	OG1	THR	1	561	-4.864	-18.913	-4.033	1.00	0.75
ATOM	309	CG2	THR	1	561	-6.811	-17.868	-3.035	1.00	0.75
ATOM	310	N	THR	1	562	-4.503	-15.997	-0.883	1.00	4.60
ATOM	311	CA	THR	1	562	-4.985	-15.299	0.272	1.00	4.60
ATOM	312	C	THR	1	562	-4.840	-13.814	0.133	1.00	4.60
ATOM	313	O	THR	1	562	-5.749	-13.078	0.514	1.00	4.60
ATOM	314	CB	THR	1	562	-4.347	-15.723	1.571	1.00	4.60
ATOM	315	OG1	THR	1	562	-5.143	-15.272	2.658	1.00	4.60
ATOM	316	CG2	THR	1	562	-2.945	-15.112	1.703	1.00	4.60
ATOM	317	N	LEU	1	563	-3.710	-13.318	-0.419	1.00	3.84
ATOM	318	CA	LEU	1	563	-3.589	-11.887	-0.483	1.00	3.84
ATOM	319	C	LEU	1	563	-4.655	-11.438	-1.412	1.00	3.84
ATOM	320	O	LEU	1	563	-5.340	-10.444	-1.182	1.00	3.84
ATOM	321	CB	LEU	1	563	-2.329	-11.312	-1.161	1.00	3.84
ATOM	322	CG	LEU	1	563	-0.992	-11.979	-0.831	1.00	3.84
ATOM	323	CD1	LEU	1	563	-0.839	-13.222	-1.707	1.00	3.84
ATOM	324	CD2	LEU	1	563	0.197	-11.014	-0.964	1.00	3.84
ATOM	325	N	ASN	1	564	-4.818	-12.207	-2.499	1.00	3.56
ATOM	326	CA	ASN	1	564	-5.696	-11.869	-3.572	1.00	3.56
ATOM	327	C	ASN	1	564	-7.113	-11.760	-3.109	1.00	3.56
ATOM	328	O	ASN	1	564	-7.853	-10.902	-3.586	1.00	3.56
ATOM	329	CB	ASN	1	564	-5.638	-12.914	-4.692	1.00	3.56
ATOM	330	CG	ASN	1	564	-6.061	-12.202	-5.953	1.00	3.56
ATOM	331	OD1	ASN	1	564	-7.106	-12.483	-6.539	1.00	3.56
ATOM	332	ND2	ASN	1	564	-5.205	-11.231	-6.370	1.00	3.56
ATOM	333	N	MET	1	565	-7.531	-12.613	-2.155	1.00	5.34
ATOM	334	CA	MET	1	565	-8.898	-12.577	-1.713	1.00	5.34
ATOM	335	C	MET	1	565	-9.213	-11.199	-1.222	1.00	5.34
ATOM	336	O	MET	1	565	-10.265	-10.646	-1.540	1.00	5.34
ATOM	337	CB	MET	1	565	-9.165	-13.522	-0.524	1.00	5.34
ATOM	338	CG	MET	1	565	-9.227	-15.013	-0.868	1.00	5.34
ATOM	339	SD	MET	1	565	-10.846	-15.587	-1.472	1.00	5.34
ATOM	340	CE	MET	1	565	-11.623	-15.702	0.166	1.00	5.34
ATOM	341	N	LEU	1	566	-8.304	-10.627	-0.412	1.00	1.68
ATOM	342	CA	LEU	1	566	-8.430	-9.317	0.170	1.00	1.68
ATOM	343	C	LEU	1	566	-8.206	-8.166	-0.760	1.00	1.68
ATOM	344	O	LEU	1	566	-8.694	-7.069	-0.497	1.00	1.68

181/208

ATOM	345	CB	LEU	1	566	-7.494	-9.071	1.368	1.00	1.68
ATOM	346	CG	LEU	1	566	-7.870	-9.869	2.628	1.00	1.68
ATOM	347	CD1	LEU	1	566	-6.977	-9.475	3.815	1.00	1.68
ATOM	348	CD2	LEU	1	566	-9.368	-9.737	2.945	1.00	1.68
ATOM	349	N	GLY	1	567	-7.446	-8.371	-1.852	1.00	1.08
ATOM	350	CA	GLY	1	567	-7.005	-7.298	-2.704	1.00	1.08
ATOM	351	C	GLY	1	567	-8.083	-6.411	-3.249	1.00	1.08
ATOM	352	O	GLY	1	567	-7.882	-5.202	-3.354	1.00	1.08
ATOM	353	N	GLY	1	568	-9.245	-6.968	-3.633	1.00	0.69
ATOM	354	CA	GLY	1	568	-10.276	-6.151	-4.209	1.00	0.69
ATOM	355	C	GLY	1	568	-10.734	-5.095	-3.250	1.00	0.69
ATOM	356	O	GLY	1	568	-10.984	-3.958	-3.637	1.00	0.69
ATOM	357	N	ARG	1	569	-10.894	-5.421	-1.963	1.00	8.50
ATOM	358	CA	ARG	1	569	-11.347	-4.412	-1.049	1.00	8.50
ATOM	359	C	ARG	1	569	-10.311	-3.332	-0.953	1.00	8.50
ATOM	360	O	ARG	1	569	-10.625	-2.143	-0.913	1.00	8.50
ATOM	361	CB	ARG	1	569	-11.586	-4.953	0.372	1.00	8.50
ATOM	362	CG	ARG	1	569	-12.843	-5.819	0.536	1.00	8.50
ATOM	363	CD	ARG	1	569	-12.824	-7.141	-0.237	1.00	8.50
ATOM	364	NE	ARG	1	569	-13.206	-6.855	-1.650	1.00	8.50
ATOM	365	CZ	ARG	1	569	-12.718	-7.634	-2.660	1.00	8.50
ATOM	366	NH1	ARG	1	569	-11.861	-8.659	-2.377	1.00	8.50
ATOM	367	NH2	ARG	1	569	-13.087	-7.391	-3.951	1.00	8.50
ATOM	368	N	GLN	1	570	-9.030	-3.730	-0.922	1.00	0.65
ATOM	369	CA	GLN	1	570	-7.957	-2.791	-0.774	1.00	0.65
ATOM	370	C	GLN	1	570	-7.918	-1.860	-1.944	1.00	0.65
ATOM	371	O	GLN	1	570	-7.699	-0.660	-1.780	1.00	0.65
ATOM	372	CB	GLN	1	570	-6.584	-3.476	-0.703	1.00	0.65
ATOM	373	CG	GLN	1	570	-6.407	-4.379	0.518	1.00	0.65
ATOM	374	CD	GLN	1	570	-5.012	-4.978	0.446	1.00	0.65
ATOM	375	OE1	GLN	1	570	-4.262	-4.718	-0.494	1.00	0.65
ATOM	376	NE2	GLN	1	570	-4.651	-5.807	1.462	1.00	0.65
ATOM	377	N	VAL	1	571	-8.116	-2.396	-3.162	1.00	4.09
ATOM	378	CA	VAL	1	571	-8.061	-1.597	-4.350	1.00	4.09
ATOM	379	C	VAL	1	571	-9.161	-0.576	-4.319	1.00	4.09
ATOM	380	O	VAL	1	571	-8.904	0.612	-4.488	1.00	4.09
ATOM	381	CB	VAL	1	571	-8.180	-2.448	-5.611	1.00	4.09
ATOM	382	CG1	VAL	1	571	-9.582	-3.028	-5.750	1.00	4.09
ATOM	383	CG2	VAL	1	571	-7.855	-1.633	-6.856	1.00	4.09
ATOM	384	N	ILE	1	572	-10.419	-0.955	-4.025	1.00	7.34
ATOM	385	CA	ILE	1	572	-11.411	0.081	-4.132	1.00	7.34
ATOM	386	C	ILE	1	572	-11.182	1.164	-3.124	1.00	7.34
ATOM	387	O	ILE	1	572	-11.483	2.326	-3.386	1.00	7.34
ATOM	388	CB	ILE	1	572	-12.868	-0.317	-4.065	1.00	7.34
ATOM	389	CG1	ILE	1	572	-13.301	-0.901	-2.715	1.00	7.34
ATOM	390	CG2	ILE	1	572	-13.127	-1.259	-5.252	1.00	7.34
ATOM	391	CD1	ILE	1	572	-12.853	-2.332	-2.490	1.00	7.34
ATOM	392	N	ALA	1	573	-10.612	0.818	-1.957	1.00	0.75
ATOM	393	CA	ALA	1	573	-10.379	1.810	-0.949	1.00	0.75
ATOM	394	C	ALA	1	573	-9.475	2.880	-1.482	1.00	0.75
ATOM	395	O	ALA	1	573	-9.693	4.063	-1.229	1.00	0.75
ATOM	396	CB	ALA	1	573	-9.718	1.230	0.313	1.00	0.75
ATOM	397	N	ALA	1	574	-8.428	2.496	-2.236	1.00	0.63
ATOM	398	CA	ALA	1	574	-7.516	3.468	-2.772	1.00	0.63
ATOM	399	C	ALA	1	574	-8.244	4.342	-3.747	1.00	0.63
ATOM	400	O	ALA	1	574	-8.018	5.549	-3.802	1.00	0.63
ATOM	401	CB	ALA	1	574	-6.310	2.829	-3.482	1.00	0.63
ATOM	402	N	VAL	1	575	-9.147	3.744	-4.550	1.00	0.59
ATOM	403	CA	VAL	1	575	-9.902	4.488	-5.519	1.00	0.59
ATOM	404	C	VAL	1	575	-10.779	5.467	-4.804	1.00	0.59
ATOM	405	O	VAL	1	575	-10.914	6.615	-5.221	1.00	0.59

182/208

ATOM	406	CB VAL 1 575	-10.806	3.616	-6.340	1.00	0.59
ATOM	407	CG1 VAL 1 575	-11.582	4.505	-7.326	1.00	0.59
ATOM	408	CG2 VAL 1 575	-9.960	2.527	-7.019	1.00	0.59
ATOM	409	N LYS 1 576	-11.392	5.025	-3.688	1.00	5.66
ATOM	410	CA LYS 1 576	-12.292	5.853	-2.937	1.00	5.66
ATOM	411	C LYS 1 576	-11.533	7.030	-2.426	1.00	5.66
ATOM	412	O LYS 1 576	-12.029	8.155	-2.424	1.00	5.66
ATOM	413	CB LYS 1 576	-12.875	5.132	-1.709	1.00	5.66
ATOM	414	CG LYS 1 576	-13.748	3.926	-2.060	1.00	5.66
ATOM	415	CD LYS 1 576	-14.972	4.279	-2.907	1.00	5.66
ATOM	416	CE LYS 1 576	-15.839	3.066	-3.254	1.00	5.66
ATOM	417	NZ LYS 1 576	-15.076	2.130	-4.109	1.00	5.66
ATOM	418	N TRP 1 577	-10.288	6.789	-1.982	1.00	0.85
ATOM	419	CA TRP 1 577	-9.473	7.831	-1.446	1.00	0.85
ATOM	420	C TRP 1 577	-9.309	8.899	-2.481	1.00	0.85
ATOM	421	O TRP 1 577	-9.578	10.076	-2.248	1.00	0.85
ATOM	422	CB TRP 1 577	-8.070	7.313	-1.085	1.00	0.85
ATOM	423	CG TRP 1 577	-7.130	8.338	-0.507	1.00	0.85
ATOM	424	CD1 TRP 1 577	-6.897	8.652	0.799	1.00	0.85
ATOM	425	CD2 TRP 1 577	-6.244	9.157	-1.286	1.00	0.85
ATOM	426	NE1 TRP 1 577	-5.917	9.608	0.878	1.00	0.85
ATOM	427	CE2 TRP 1 577	-5.505	9.931	-0.393	1.00	0.85
ATOM	428	CE3 TRP 1 577	-6.055	9.251	-2.634	1.00	0.85
ATOM	429	CZ2 TRP 1 577	-4.570	10.822	-0.833	1.00	0.85
ATOM	430	CZ3 TRP 1 577	-5.108	10.150	-3.074	1.00	0.85
ATOM	431	CH2 TRP 1 577	-4.381	10.922	-2.193	1.00	0.85
ATOM	432	N ALA 1 578	-8.926	8.508	-3.699	1.00	1.04
ATOM	433	CA ALA 1 578	-8.660	9.480	-4.717	1.00	1.04
ATOM	434	C ALA 1 578	-9.883	10.278	-5.039	1.00	1.04
ATOM	435	O ALA 1 578	-9.799	11.479	-5.289	1.00	1.04
ATOM	436	CB ALA 1 578	-8.169	8.837	-6.026	1.00	1.04
ATOM	437	N LYS 1 579	-11.062	9.636	-5.045	1.00	4.62
ATOM	438	CA LYS 1 579	-12.259	10.335	-5.412	1.00	4.62
ATOM	439	C LYS 1 579	-12.592	11.437	-4.454	1.00	4.62
ATOM	440	O LYS 1 579	-13.125	12.471	-4.855	1.00	4.62
ATOM	441	CB LYS 1 579	-13.477	9.411	-5.561	1.00	4.62
ATOM	442	CG LYS 1 579	-13.391	8.576	-6.839	1.00	4.62
ATOM	443	CD LYS 1 579	-14.419	7.452	-6.939	1.00	4.62
ATOM	444	CE LYS 1 579	-14.310	6.661	-8.245	1.00	4.62
ATOM	445	NZ LYS 1 579	-14.577	7.549	-9.399	1.00	4.62
ATOM	446	N ALA 1 580	-12.288	11.248	-3.159	1.00	1.29
ATOM	447	CA ALA 1 580	-12.598	12.223	-2.151	1.00	1.29
ATOM	448	C ALA 1 580	-11.822	13.493	-2.321	1.00	1.29
ATOM	449	O ALA 1 580	-12.196	14.518	-1.753	1.00	1.29
ATOM	450	CB ALA 1 580	-12.371	11.733	-0.717	1.00	1.29
ATOM	451	N ILE 1 581	-10.682	13.451	-3.042	1.00	3.84
ATOM	452	CA ILE 1 581	-9.885	14.636	-3.206	1.00	3.84
ATOM	453	C ILE 1 581	-10.346	15.411	-4.410	1.00	3.84
ATOM	454	O ILE 1 581	-10.388	14.917	-5.536	1.00	3.84
ATOM	455	CB ILE 1 581	-8.415	14.317	-3.325	1.00	3.84
ATOM	456	CG1 ILE 1 581	-7.541	15.562	-3.135	1.00	3.84
ATOM	457	CG2 ILE 1 581	-8.166	13.584	-4.651	1.00	3.84
ATOM	458	CD1 ILE 1 581	-6.071	15.199	-2.925	1.00	3.84
ATOM	459	N PRO 1 582	-10.712	16.640	-4.160	1.00	3.26
ATOM	460	CA PRO 1 582	-11.266	17.522	-5.155	1.00	3.26
ATOM	461	C PRO 1 582	-10.417	17.677	-6.381	1.00	3.26
ATOM	462	O PRO 1 582	-10.967	17.695	-7.481	1.00	3.26
ATOM	463	CB PRO 1 582	-11.447	18.862	-4.446	1.00	3.26
ATOM	464	CG PRO 1 582	-10.333	18.851	-3.381	1.00	3.26
ATOM	465	CD PRO 1 582	-10.191	17.365	-3.012	1.00	3.26
ATOM	466	N GLY 1 583	-9.088	17.794	-6.227	1.00	0.75



183/208

ATOM	467	CA	GLY 1 583	-8.238	18.027	-7.358	1.00	0.75
ATOM	468	C	GLY 1 583	-8.296	16.878	-8.311	1.00	0.75
ATOM	469	O	GLY 1 583	-8.201	17.067	-9.521	1.00	0.75
ATOM	470	N	PHE 1 584	-8.420	15.655	-7.768	1.00	1.03
ATOM	471	CA	PHE 1 584	-8.409	14.430	-8.520	1.00	1.03
ATOM	472	C	PHE 1 584	-9.581	14.306	-9.446	1.00	1.03
ATOM	473	O	PHE 1 584	-9.430	13.931	-10.608	1.00	1.03
ATOM	474	CB	PHE 1 584	-8.422	13.217	-7.568	1.00	1.03
ATOM	475	CG	PHE 1 584	-8.361	11.929	-8.319	1.00	1.03
ATOM	476	CD1	PHE 1 584	-7.161	11.470	-8.810	1.00	1.03
ATOM	477	CD2	PHE 1 584	-9.444	11.078	-8.324	1.00	1.03
ATOM	478	CE1	PHE 1 584	-7.049	10.201	-9.329	1.00	1.03
ATOM	479	CE2	PHE 1 584	-9.337	9.805	-8.837	1.00	1.03
ATOM	480	CZ	PHE 1 584	-8.134	9.359	-9.328	1.00	1.03
ATOM	481	N	ARG 1 585	-10.782	14.653	-8.951	1.00	5.26
ATOM	482	CA	ARG 1 585	-11.990	14.486	-9.706	1.00	5.26
ATOM	483	C	ARG 1 585	-11.955	15.324	-10.940	1.00	5.26
ATOM	484	O	ARG 1 585	-12.483	14.934	-11.980	1.00	5.26
ATOM	485	CB	ARG 1 585	-13.247	14.881	-8.912	1.00	5.26
ATOM	486	CG	ARG 1 585	-14.548	14.666	-9.688	1.00	5.26
ATOM	487	CD	ARG 1 585	-15.802	15.056	-8.904	1.00	5.26
ATOM	488	NE	ARG 1 585	-16.977	14.796	-9.784	1.00	5.26
ATOM	489	CZ	ARG 1 585	-18.231	14.750	-9.249	1.00	5.26
ATOM	490	NH1	ARG 1 585	-19.307	14.502	-10.052	1.00	5.26
ATOM	491	NH2	ARG 1 585	-18.411	14.954	-7.910	1.00	5.26
ATOM	492	N	ASN 1 586	-11.322	16.506	-10.856	1.00	0.91
ATOM	493	CA	ASN 1 586	-11.280	17.411	-11.966	1.00	0.91
ATOM	494	C	ASN 1 586	-10.596	16.779	-13.138	1.00	0.91
ATOM	495	O	ASN 1 586	-10.973	17.026	-14.282	1.00	0.91
ATOM	496	CB	ASN 1 586	-10.529	18.714	-11.645	1.00	0.91
ATOM	497	CG	ASN 1 586	-11.381	19.523	-10.676	1.00	0.91
ATOM	498	OD1	ASN 1 586	-12.586	19.670	-10.867	1.00	0.91
ATOM	499	ND2	ASN 1 586	-10.739	20.060	-9.604	1.00	0.91
ATOM	500	N	LEU 1 587	-9.569	15.947	-12.892	1.00	4.04
ATOM	501	CA	LEU 1 587	-8.834	15.380	-13.988	1.00	4.04
ATOM	502	C	LEU 1 587	-9.724	14.592	-14.891	1.00	4.04
ATOM	503	O	LEU 1 587	-10.793	14.129	-14.499	1.00	4.04
ATOM	504	CB	LEU 1 587	-7.698	14.425	-13.571	1.00	4.04
ATOM	505	CG	LEU 1 587	-6.611	15.067	-12.690	1.00	4.04
ATOM	506	CD1	LEU 1 587	-7.107	15.257	-11.255	1.00	4.04
ATOM	507	CD2	LEU 1 587	-5.287	14.295	-12.751	1.00	4.04
ATOM	508	N	HIS 1 588	-9.290	14.422	-16.155	1.00	3.17
ATOM	509	CA	HIS 1 588	-10.079	13.664	-17.076	1.00	3.17
ATOM	510	C	HIS 1 588	-10.007	12.242	-16.633	1.00	3.17
ATOM	511	O	HIS 1 588	-9.091	11.842	-15.917	1.00	3.17
ATOM	512	CB	HIS 1 588	-9.598	13.754	-18.533	1.00	3.17
ATOM	513	CG	HIS 1 588	-9.688	15.146	-19.088	1.00	3.17
ATOM	514	ND1	HIS 1 588	-8.713	16.103	-18.921	1.00	3.17
ATOM	515	CD2	HIS 1 588	-10.655	15.730	-19.848	1.00	3.17
ATOM	516	CE1	HIS 1 588	-9.134	17.211	-19.581	1.00	3.17
ATOM	517	NE2	HIS 1 588	-10.309	17.033	-20.159	1.00	3.17
ATOM	518	N	LEU 1 589	-10.986	11.432	-17.066	1.00	6.31
ATOM	519	CA	LEU 1 589	-11.066	10.071	-16.633	1.00	6.31
ATOM	520	C	LEU 1 589	-9.832	9.331	-17.025	1.00	6.31
ATOM	521	O	LEU 1 589	-9.335	8.501	-16.267	1.00	6.31
ATOM	522	CB	LEU 1 589	-12.264	9.322	-17.240	1.00	6.31
ATOM	523	CG	LEU 1 589	-12.366	7.856	-16.779	1.00	6.31
ATOM	524	CD1	LEU 1 589	-12.605	7.759	-15.265	1.00	6.31
ATOM	525	CD2	LEU 1 589	-13.414	7.086	-17.599	1.00	6.31
ATOM	526	N	ASP 1 590	-9.298	9.614	-18.224	1.00	4.07
ATOM	527	CA	ASP 1 590	-8.153	8.874	-18.669	1.00	4.07

184/208

ATOM	528	C	ASP	1	590	-6.992	9.057	-17.744	1.00	4.07
ATOM	529	O	ASP	1	590	-6.344	8.084	-17.365	1.00	4.07
ATOM	530	CB	ASP	1	590	-7.704	9.236	-20.099	1.00	4.07
ATOM	531	CG	ASP	1	590	-7.307	10.703	-20.151	1.00	4.07
ATOM	532	OD1	ASP	1	590	-7.873	11.496	-19.353	1.00	4.07
ATOM	533	OD2	ASP	1	590	-6.436	11.053	-20.992	1.00	4.07
ATOM	534	N	ASP	1	591	-6.691	10.304	-17.343	1.00	5.67
ATOM	535	CA	ASP	1	591	-5.581	10.496	-16.462	1.00	5.67
ATOM	536	C	ASP	1	591	-5.860	9.994	-15.078	1.00	5.67
ATOM	537	O	ASP	1	591	-4.955	9.560	-14.366	1.00	5.67
ATOM	538	CB	ASP	1	591	-4.982	11.914	-16.507	1.00	5.67
ATOM	539	CG	ASP	1	591	-6.017	12.981	-16.269	1.00	5.67
ATOM	540	OD1	ASP	1	591	-5.748	13.867	-15.419	1.00	5.67
ATOM	541	OD2	ASP	1	591	-7.067	12.957	-16.959	1.00	5.67
ATOM	542	N	GLN	1	592	-7.139	10.019	-14.668	1.00	3.91
ATOM	543	CA	GLN	1	592	-7.529	9.540	-13.376	1.00	3.91
ATOM	544	C	GLN	1	592	-7.134	8.098	-13.282	1.00	3.91
ATOM	545	O	GLN	1	592	-6.576	7.658	-12.277	1.00	3.91
ATOM	546	CB	GLN	1	592	-9.055	9.639	-13.213	1.00	3.91
ATOM	547	CG	GLN	1	592	-9.601	9.161	-11.873	1.00	3.91
ATOM	548	CD	GLN	1	592	-11.113	9.338	-11.900	1.00	3.91
ATOM	549	OE1	GLN	1	592	-11.867	8.413	-11.598	1.00	3.91
ATOM	550	NE2	GLN	1	592	-11.574	10.564	-12.269	1.00	3.91
ATOM	551	N	MET	1	593	-7.404	7.323	-14.351	1.00	7.01
ATOM	552	CA	MET	1	593	-7.112	5.919	-14.356	1.00	7.01
ATOM	553	C	MET	1	593	-5.636	5.669	-14.286	1.00	7.01
ATOM	554	O	MET	1	593	-5.177	4.839	-13.503	1.00	7.01
ATOM	555	CB	MET	1	593	-7.648	5.216	-15.618	1.00	7.01
ATOM	556	CG	MET	1	593	-7.623	3.686	-15.552	1.00	7.01
ATOM	557	SD	MET	1	593	-5.971	2.929	-15.626	1.00	7.01
ATOM	558	CE	MET	1	593	-6.578	1.220	-15.511	1.00	7.01
ATOM	559	N	THR	1	594	-4.845	6.403	-15.092	1.00	0.78
ATOM	560	CA	THR	1	594	-3.429	6.170	-15.146	1.00	0.78
ATOM	561	C	THR	1	594	-2.828	6.465	-13.814	1.00	0.78
ATOM	562	O	THR	1	594	-1.933	5.772	-13.335	1.00	0.78
ATOM	563	CB	THR	1	594	-2.739	7.045	-16.151	1.00	0.78
ATOM	564	OG1	THR	1	594	-3.268	6.813	-17.448	1.00	0.78
ATOM	565	CG2	THR	1	594	-1.234	6.727	-16.129	1.00	0.78
ATOM	566	N	LEU	1	595	-3.332	7.530	-13.187	1.00	6.73
ATOM	567	CA	LEU	1	595	-2.861	8.039	-11.943	1.00	6.73
ATOM	568	C	LEU	1	595	-3.069	7.019	-10.875	1.00	6.73
ATOM	569	O	LEU	1	595	-2.176	6.702	-10.090	1.00	6.73
ATOM	570	CB	LEU	1	595	-3.723	9.246	-11.624	1.00	6.73
ATOM	571	CG	LEU	1	595	-3.056	10.184	-10.664	1.00	6.73
ATOM	572	CD1	LEU	1	595	-1.680	10.521	-11.250	1.00	6.73
ATOM	573	CD2	LEU	1	595	-3.970	11.395	-10.435	1.00	6.73
ATOM	574	N	LEU	1	596	-4.286	6.462	-10.859	1.00	6.22
ATOM	575	CA	LEU	1	596	-4.726	5.531	-9.876	1.00	6.22
ATOM	576	C	LEU	1	596	-3.874	4.315	-10.036	1.00	6.22
ATOM	577	O	LEU	1	596	-3.404	3.721	-9.067	1.00	6.22
ATOM	578	CB	LEU	1	596	-6.201	5.209	-10.157	1.00	6.22
ATOM	579	CG	LEU	1	596	-6.995	4.659	-8.972	1.00	6.22
ATOM	580	CD1	LEU	1	596	-7.054	5.683	-7.827	1.00	6.22
ATOM	581	CD2	LEU	1	596	-8.393	4.211	-9.414	1.00	6.22
ATOM	582	N	GLN	1	597	-3.624	3.936	-11.296	1.00	3.34
ATOM	583	CA	GLN	1	597	-2.857	2.764	-11.591	1.00	3.34
ATOM	584	C	GLN	1	597	-1.445	2.904	-11.116	1.00	3.34
ATOM	585	O	GLN	1	597	-0.871	1.959	-10.580	1.00	3.34
ATOM	586	CB	GLN	1	597	-2.806	2.471	-13.097	1.00	3.34
ATOM	587	CG	GLN	1	597	-1.995	1.225	-13.456	1.00	3.34
ATOM	588	CD	GLN	1	597	-2.036	1.069	-14.968	1.00	3.34

185/208

ATOM	589	OE1 GLN 1 597	-3.114	1.065	-15.570	1.00	3.34
ATOM	590	NE2 GLN 1 597	-0.844	0.946	-15.606	1.00	3.34
ATOM	591	N TYR 1 598	-0.840	4.086	-11.323	1.00	7.16
ATOM	592	CA TYR 1 598	0.539	4.275	-10.976	1.00	7.16
ATOM	593	C TYR 1 598	0.810	4.257	-9.501	1.00	7.16
ATOM	594	O TYR 1 598	1.769	3.635	-9.051	1.00	7.16
ATOM	595	CB TYR 1 598	1.093	5.591	-11.532	1.00	7.16
ATOM	596	CG TYR 1 598	2.525	5.717	-11.138	1.00	7.16
ATOM	597	CD1 TYR 1 598	3.517	5.120	-11.883	1.00	7.16
ATOM	598	CD2 TYR 1 598	2.881	6.510	-10.073	1.00	7.16
ATOM	599	CE1 TYR 1 598	4.842	5.306	-11.566	1.00	7.16
ATOM	600	CE2 TYR 1 598	4.205	6.712	-9.763	1.00	7.16
ATOM	601	CZ TYR 1 598	5.188	6.108	-10.506	1.00	7.16
ATOM	602	OH TYR 1 598	6.547	6.317	-10.185	1.00	7.16
ATOM	603	N SER 1 599	-0.013	4.975	-8.716	1.00	4.48
ATOM	604	CA SER 1 599	0.146	5.134	-7.293	1.00	4.48
ATOM	605	C SER 1 599	-0.364	3.986	-6.474	1.00	4.48
ATOM	606	O SER 1 599	-0.056	3.853	-5.291	1.00	4.48
ATOM	607	CB SER 1 599	-0.501	6.433	-6.784	1.00	4.48
ATOM	608	OG SER 1 599	0.029	6.770	-5.511	1.00	4.48
ATOM	609	N TRP 1 600	-1.166	3.123	-7.103	1.00	2.83
ATOM	610	CA TRP 1 600	-1.945	2.101	-6.479	1.00	2.83
ATOM	611	C TRP 1 600	-1.188	1.302	-5.467	1.00	2.83
ATOM	612	O TRP 1 600	-1.561	1.258	-4.294	1.00	2.83
ATOM	613	CB TRP 1 600	-2.341	1.109	-7.565	1.00	2.83
ATOM	614	CG TRP 1 600	-3.591	0.441	-7.181	1.00	2.83
ATOM	615	CD1 TRP 1 600	-3.942	-0.815	-6.793	1.00	2.83
ATOM	616	CD2 TRP 1 600	-4.693	1.293	-6.907	1.00	2.83
ATOM	617	NE1 TRP 1 600	-5.257	-0.809	-6.409	1.00	2.83
ATOM	618	CE2 TRP 1 600	-5.718	0.492	-6.479	1.00	2.83
ATOM	619	CE3 TRP 1 600	-4.818	2.647	-6.992	1.00	2.83
ATOM	620	CZ2 TRP 1 600	-6.916	1.047	-6.205	1.00	2.83
ATOM	621	CZ3 TRP 1 600	-6.018	3.201	-6.627	1.00	2.83
ATOM	622	CH2 TRP 1 600	-7.081	2.405	-6.290	1.00	2.83
ATOM	623	N MET 1 601	-0.100	0.641	-5.888	1.00	4.56
ATOM	624	CA MET 1 601	0.614	-0.167	-4.950	1.00	4.56
ATOM	625	C MET 1 601	1.324	0.717	-3.974	1.00	4.56
ATOM	626	O MET 1 601	1.564	0.322	-2.836	1.00	4.56
ATOM	627	CB MET 1 601	1.602	-1.163	-5.582	1.00	4.56
ATOM	628	CG MET 1 601	3.025	-0.654	-5.783	1.00	4.56
ATOM	629	SD MET 1 601	4.060	-0.617	-4.285	1.00	4.56
ATOM	630	CE MET 1 601	4.167	-2.419	-4.091	1.00	4.56
ATOM	631	N PHE 1 602	1.706	1.937	-4.408	1.00	6.98
ATOM	632	CA PHE 1 602	2.410	2.844	-3.542	1.00	6.98
ATOM	633	C PHE 1 602	1.582	3.074	-2.317	1.00	6.98
ATOM	634	O PHE 1 602	2.086	2.981	-1.200	1.00	6.98
ATOM	635	CB PHE 1 602	2.534	4.278	-4.096	1.00	6.98
ATOM	636	CG PHE 1 602	3.498	4.431	-5.217	1.00	6.98
ATOM	637	CD1 PHE 1 602	3.158	4.051	-6.495	1.00	6.98
ATOM	638	CD2 PHE 1 602	4.567	5.281	-5.046	1.00	6.98
ATOM	639	CE1 PHE 1 602	3.924	4.447	-7.564	1.00	6.98
ATOM	640	CE2 PHE 1 602	5.340	5.673	-6.109	1.00	6.98
ATOM	641	CZ PHE 1 602	5.042	5.221	-7.369	1.00	6.98
ATOM	642	N LEU 1 603	0.286	3.407	-2.501	1.00	3.79
ATOM	643	CA LEU 1 603	-0.551	3.686	-1.365	1.00	3.79
ATOM	644	C LEU 1 603	-0.740	2.459	-0.541	1.00	3.79
ATOM	645	O LEU 1 603	-0.676	2.509	0.685	1.00	3.79
ATOM	646	CB LEU 1 603	-1.995	4.128	-1.677	1.00	3.79
ATOM	647	CG LEU 1 603	-2.165	5.496	-2.352	1.00	3.79
ATOM	648	CD1 LEU 1 603	-1.536	6.626	-1.521	1.00	3.79
ATOM	649	CD2 LEU 1 603	-1.720	5.453	-3.813	1.00	3.79

186/208

ATOM	650	N	MET	1	604	-0.978	1.317	-1.209	1.00	5.17
ATOM	651	CA	MET	1	604	-1.284	0.101	-0.519	1.00	5.17
ATOM	652	C	MET	1	604	-0.137	-0.248	0.370	1.00	5.17
ATOM	653	O	MET	1	604	-0.322	-0.589	1.537	1.00	5.17
ATOM	654	CB	MET	1	604	-1.430	-1.091	-1.479	1.00	5.17
ATOM	655	CG	MET	1	604	-2.428	-0.856	-2.612	1.00	5.17
ATOM	656	SD	MET	1	604	-4.150	-0.604	-2.106	1.00	5.17
ATOM	657	CE	MET	1	604	-4.639	-0.119	-3.784	1.00	5.17
ATOM	658	N	ALA	1	605	1.090	-0.153	-0.170	1.00	0.70
ATOM	659	CA	ALA	1	605	2.263	-0.519	0.565	1.00	0.70
ATOM	660	C	ALA	1	605	2.414	0.368	1.754	1.00	0.70
ATOM	661	O	ALA	1	605	2.793	-0.090	2.830	1.00	0.70
ATOM	662	CB	ALA	1	605	3.551	-0.397	-0.268	1.00	0.70
ATOM	663	N	PHE	1	606	2.133	1.673	1.590	1.00	4.22
ATOM	664	CA	PHE	1	606	2.309	2.548	2.707	1.00	4.22
ATOM	665	C	PHE	1	606	1.317	2.211	3.776	1.00	4.22
ATOM	666	O	PHE	1	606	1.648	2.206	4.960	1.00	4.22
ATOM	667	CB	PHE	1	606	2.157	4.042	2.396	1.00	4.22
ATOM	668	CG	PHE	1	606	2.785	4.728	3.563	1.00	4.22
ATOM	669	CD1	PHE	1	606	2.099	4.905	4.743	1.00	4.22
ATOM	670	CD2	PHE	1	606	4.109	5.095	3.513	1.00	4.22
ATOM	671	CE1	PHE	1	606	2.706	5.477	5.835	1.00	4.22
ATOM	672	CE2	PHE	1	606	4.725	5.668	4.600	1.00	4.22
ATOM	673	CZ	PHE	1	606	4.022	5.863	5.765	1.00	4.22
ATOM	674	N	ALA	1	607	0.069	1.893	3.381	1.00	0.92
ATOM	675	CA	ALA	1	607	-0.960	1.605	4.338	1.00	0.92
ATOM	676	C	ALA	1	607	-0.537	0.427	5.153	1.00	0.92
ATOM	677	O	ALA	1	607	-0.765	0.376	6.361	1.00	0.92
ATOM	678	CB	ALA	1	607	-2.302	1.253	3.676	1.00	0.92
ATOM	679	N	LEU	1	608	0.067	-0.568	4.487	1.00	4.26
ATOM	680	CA	LEU	1	608	0.559	-1.747	5.129	1.00	4.26
ATOM	681	C	LEU	1	608	1.704	-1.393	6.034	1.00	4.26
ATOM	682	O	LEU	1	608	1.779	-1.876	7.161	1.00	4.26
ATOM	683	CB	LEU	1	608	1.010	-2.780	4.068	1.00	4.26
ATOM	684	CG	LEU	1	608	1.578	-4.119	4.573	1.00	4.26
ATOM	685	CD1	LEU	1	608	1.752	-5.104	3.410	1.00	4.26
ATOM	686	CD2	LEU	1	608	2.921	-3.927	5.286	1.00	4.26
ATOM	687	N	GLY	1	609	2.631	-0.542	5.551	1.00	0.62
ATOM	688	CA	GLY	1	609	3.824	-0.209	6.281	1.00	0.62
ATOM	689	C	GLY	1	609	3.521	0.478	7.577	1.00	0.62
ATOM	690	O	GLY	1	609	4.164	0.210	8.589	1.00	0.62
ATOM	691	N	TRP	1	610	2.542	1.395	7.598	1.00	3.39
ATOM	692	CA	TRP	1	610	2.246	2.087	8.821	1.00	3.39
ATOM	693	C	TRP	1	610	1.768	1.108	9.843	1.00	3.39
ATOM	694	O	TRP	1	610	1.936	1.305	11.045	1.00	3.39
ATOM	695	CB	TRP	1	610	1.172	3.178	8.672	1.00	3.39
ATOM	696	CG	TRP	1	610	0.730	3.769	9.990	1.00	3.39
ATOM	697	CD1	TRP	1	610	-0.435	3.565	10.671	1.00	3.39
ATOM	698	CD2	TRP	1	610	1.575	4.541	10.858	1.00	3.39
ATOM	699	NE1	TRP	1	610	-0.391	4.210	11.884	1.00	3.39
ATOM	700	CE2	TRP	1	610	0.846	4.805	12.018	1.00	3.39
ATOM	701	CE3	TRP	1	610	2.860	4.981	10.709	1.00	3.39
ATOM	702	CZ2	TRP	1	610	1.388	5.525	13.044	1.00	3.39
ATOM	703	CZ3	TRP	1	610	3.408	5.692	11.754	1.00	3.39
ATOM	704	CH2	TRP	1	610	2.684	5.966	12.895	1.00	3.39
ATOM	705	N	ARG	1	611	1.110	0.045	9.366	1.00	4.02
ATOM	706	CA	ARG	1	611	0.550	-1.005	10.161	1.00	4.02
ATOM	707	C	ARG	1	611	1.493	-2.017	10.738	1.00	4.02
ATOM	708	O	ARG	1	611	1.046	-2.871	11.500	1.00	4.02
ATOM	709	CB	ARG	1	611	-0.632	-1.729	9.497	1.00	4.02
ATOM	710	CG	ARG	1	611	-1.429	-0.764	8.613	1.00	4.02

187/208

ATOM	711	CD	ARG	1	611	-2.571	-1.408	7.827	1.00	4.02
ATOM	712	NE	ARG	1	611	-1.971	-2.364	6.856	1.00	4.02
ATOM	713	CZ	ARG	1	611	-2.100	-2.115	5.520	1.00	4.02
ATOM	714	NH1	ARG	1	611	-2.768	-1.002	5.099	1.00	4.02
ATOM	715	NH2	ARG	1	611	-1.570	-2.977	4.605	1.00	4.02
ATOM	716	N	SER	1	612	2.787	-2.048	10.363	1.00	4.05
ATOM	717	CA	SER	1	612	3.539	-3.105	10.979	1.00	4.05
ATOM	718	C	SER	1	612	3.668	-2.931	12.454	1.00	4.05
ATOM	719	O	SER	1	612	3.685	-1.817	12.976	1.00	4.05
ATOM	720	CB	SER	1	612	4.919	-3.410	10.387	1.00	4.05
ATOM	721	OG	SER	1	612	5.539	-4.473	11.094	1.00	4.05
ATOM	722	N	TYR	1	613	3.743	-4.074	13.163	1.00	4.51
ATOM	723	CA	TYR	1	613	3.792	-4.072	14.594	1.00	4.51
ATOM	724	C	TYR	1	613	5.133	-4.616	14.963	1.00	4.51
ATOM	725	O	TYR	1	613	5.519	-5.697	14.522	1.00	4.51
ATOM	726	CB	TYR	1	613	2.716	-4.995	15.193	1.00	4.51
ATOM	727	CG	TYR	1	613	2.510	-4.676	16.633	1.00	4.51
ATOM	728	CD1	TYR	1	613	3.337	-5.181	17.606	1.00	4.51
ATOM	729	CD2	TYR	1	613	1.402	-3.951	17.009	1.00	4.51
ATOM	730	CE1	TYR	1	613	3.064	-4.947	18.934	1.00	4.51
ATOM	731	CE2	TYR	1	613	1.125	-3.716	18.335	1.00	4.51
ATOM	732	CZ	TYR	1	613	1.959	-4.221	19.302	1.00	4.51
ATOM	733	OH	TYR	1	613	1.675	-4.003	20.667	1.00	4.51
ATOM	734	N	ARG	1	614	5.891	-3.866	15.783	1.00	6.30
ATOM	735	CA	ARG	1	614	7.211	-4.286	16.147	1.00	6.30
ATOM	736	C	ARG	1	614	7.154	-5.564	16.919	1.00	6.30
ATOM	737	O	ARG	1	614	7.863	-6.520	16.608	1.00	6.30
ATOM	738	CB	ARG	1	614	7.917	-3.260	17.047	1.00	6.30
ATOM	739	CG	ARG	1	614	8.166	-1.916	16.361	1.00	6.30
ATOM	740	CD	ARG	1	614	6.880	-1.217	15.918	1.00	6.30
ATOM	741	NE	ARG	1	614	6.009	-1.054	17.116	1.00	6.30
ATOM	742	CZ	ARG	1	614	4.734	-0.591	16.966	1.00	6.30
ATOM	743	NH1	ARG	1	614	4.264	-0.277	15.724	1.00	6.30
ATOM	744	NH2	ARG	1	614	3.928	-0.444	18.057	1.00	6.30
ATOM	745	N	GLN	1	615	6.284	-5.619	17.943	1.00	3.13
ATOM	746	CA	GLN	1	615	6.219	-6.789	18.769	1.00	3.13
ATOM	747	C	GLN	1	615	5.740	-7.940	17.956	1.00	3.13
ATOM	748	O	GLN	1	615	6.283	-9.042	18.030	1.00	3.13
ATOM	749	CB	GLN	1	615	5.251	-6.635	19.952	1.00	3.13
ATOM	750	CG	GLN	1	615	5.665	-5.548	20.943	1.00	3.13
ATOM	751	CD	GLN	1	615	6.925	-6.023	21.650	1.00	3.13
ATOM	752	OE1	GLN	1	615	7.457	-7.089	21.342	1.00	3.13
ATOM	753	NE2	GLN	1	615	7.419	-5.214	22.625	1.00	3.13
ATOM	754	N	SER	1	616	4.708	-7.696	17.134	1.00	4.46
ATOM	755	CA	SER	1	616	4.133	-8.738	16.345	1.00	4.46
ATOM	756	C	SER	1	616	5.206	-9.213	15.424	1.00	4.46
ATOM	757	O	SER	1	616	5.342	-10.416	15.200	1.00	4.46
ATOM	758	CB	SER	1	616	2.943	-8.225	15.520	1.00	4.46
ATOM	759	OG	SER	1	616	2.192	-9.316	15.016	1.00	4.46
ATOM	760	N	SER	1	617	5.978	-8.253	14.871	1.00	6.06
ATOM	761	CA	SER	1	617	7.119	-8.454	14.019	1.00	6.06
ATOM	762	C	SER	1	617	7.082	-7.438	12.943	1.00	6.06
ATOM	763	O	SER	1	617	6.016	-7.070	12.454	1.00	6.06
ATOM	764	CB	SER	1	617	7.235	-9.826	13.321	1.00	6.06
ATOM	765	OG	SER	1	617	7.691	-10.813	14.235	1.00	6.06
ATOM	766	N	ALA	1	618	8.272	-6.952	12.548	1.00	1.34
ATOM	767	CA	ALA	1	618	8.328	-6.034	11.458	1.00	1.34
ATOM	768	C	ALA	1	618	7.780	-6.872	10.363	1.00	1.34
ATOM	769	O	ALA	1	618	7.040	-6.399	9.503	1.00	1.34
ATOM	770	CB	ALA	1	618	9.763	-5.633	11.080	1.00	1.34
ATOM	771	N	ASN	1	619	8.117	-8.172	10.420	1.00	2.27

188/208

ATOM	772	CA	ASN 1 619	7.655	-9.121	9.458	1.00	2.27
ATOM	773	C	ASN 1 619	6.170	-9.004	9.485	1.00	2.27
ATOM	774	O	ASN 1 619	5.521	-8.973	8.442	1.00	2.27
ATOM	775	CB	ASN 1 619	7.978	-10.575	9.852	1.00	2.27
ATOM	776	CG	ASN 1 619	9.489	-10.762	9.929	1.00	2.27
ATOM	777	OD1	ASN 1 619	8.505	-11.245	10.491	1.00	2.27
ATOM	778	ND2	ASN 1 619	9.749	-9.835	8.973	1.00	2.27
ATOM	779	N	LEU 1 620	5.590	-8.915	10.698	1.00	1.42
ATOM	780	CA	LEU 1 620	4.167	-8.832	10.788	1.00	1.42
ATOM	781	C	LEU 1 620	3.676	-7.466	10.447	1.00	1.42
ATOM	782	O	LEU 1 620	3.870	-6.484	11.166	1.00	1.42
ATOM	783	CB	LEU 1 620	3.611	-9.328	12.134	1.00	1.42
ATOM	784	CG	LEU 1 620	3.876	-10.842	12.293	1.00	1.42
ATOM	785	CD1	LEU 1 620	3.339	-11.415	13.612	1.00	1.42
ATOM	786	CD2	LEU 1 620	3.363	-11.618	11.071	1.00	1.42
ATOM	787	N	LEU 1 621	3.019	-7.413	9.278	1.00	1.28
ATOM	788	CA	LEU 1 621	2.463	-6.252	8.661	1.00	1.28
ATOM	789	C	LEU 1 621	1.007	-6.575	8.629	1.00	1.28
ATOM	790	O	LEU 1 621	0.629	-7.744	8.704	1.00	1.28
ATOM	791	CB	LEU 1 621	2.927	-6.155	7.203	1.00	1.28
ATOM	792	CG	LEU 1 621	4.463	-6.148	7.063	1.00	1.28
ATOM	793	CD1	LEU 1 621	4.910	-6.052	5.593	1.00	1.28
ATOM	794	CD2	LEU 1 621	5.093	-5.062	7.948	1.00	1.28
ATOM	795	N	CYS 1 622	0.131	-5.561	8.548	1.00	1.26
ATOM	796	CA	CYS 1 622	-1.253	-5.921	8.517	1.00	1.26
ATOM	797	C	CYS 1 622	-1.831	-5.468	7.213	1.00	1.26
ATOM	798	O	CYS 1 622	-1.836	-4.277	6.907	1.00	1.26
ATOM	799	CB	CYS 1 622	-2.053	-5.269	9.652	1.00	1.26
ATOM	800	SG	CYS 1 622	-3.717	-5.966	9.791	1.00	1.26
ATOM	801	N	PHE 1 623	-2.346	-6.415	6.402	1.00	4.97
ATOM	802	CA	PHE 1 623	-2.922	-6.047	5.139	1.00	4.97
ATOM	803	C	PHE 1 623	-4.365	-5.819	5.378	1.00	4.97
ATOM	804	O	PHE 1 623	-4.995	-6.711	5.951	1.00	4.97
ATOM	805	CB	PHE 1 623	-2.879	-7.140	4.054	1.00	4.97
ATOM	806	CG	PHE 1 623	-1.505	-7.278	3.496	1.00	4.97
ATOM	807	CD1	PHE 1 623	-0.586	-8.126	4.069	1.00	4.97
ATOM	808	CD2	PHE 1 623	-1.182	-6.645	2.317	1.00	4.97
ATOM	809	CE1	PHE 1 623	0.634	-8.337	3.468	1.00	4.97
ATOM	810	CE2	PHE 1 623	0.040	-6.846	1.721	1.00	4.97
ATOM	811	CZ	PHE 1 623	0.946	-7.707	2.290	1.00	4.97
ATOM	812	N	ALA 1 624	-4.872	-4.641	4.901	1.00	5.16
ATOM	813	CA	ALA 1 624	-6.224	-4.152	5.033	1.00	5.16
ATOM	814	C	ALA 1 624	-6.657	-4.675	6.332	1.00	5.16
ATOM	815	O	ALA 1 624	-7.324	-5.698	6.295	1.00	5.16
ATOM	816	CB	ALA 1 624	-7.182	-4.694	3.959	1.00	5.16
ATOM	817	N	PRO 1 625	-6.437	-3.914	7.376	1.00	4.05
ATOM	818	CA	PRO 1 625	-6.315	-4.317	8.776	1.00	4.05
ATOM	819	C	PRO 1 625	-6.730	-5.645	9.373	1.00	4.05
ATOM	820	O	PRO 1 625	-6.476	-5.826	10.559	1.00	4.05
ATOM	821	CB	PRO 1 625	-6.868	-3.160	9.606	1.00	4.05
ATOM	822	CG	PRO 1 625	-7.701	-2.347	8.614	1.00	4.05
ATOM	823	CD	PRO 1 625	-7.007	-2.584	7.272	1.00	4.05
ATOM	824	N	ASP 1 626	-7.415	-6.545	8.659	1.00	3.31
ATOM	825	CA	ASP 1 626	-7.765	-7.863	9.076	1.00	3.31
ATOM	826	C	ASP 1 626	-6.607	-8.827	9.191	1.00	3.31
ATOM	827	O	ASP 1 626	-6.482	-9.506	10.208	1.00	3.31
ATOM	828	CB	ASP 1 626	-8.752	-8.509	8.092	1.00	3.31
ATOM	829	CG	ASP 1 626	-10.028	-7.681	8.097	1.00	3.31
ATOM	830	OD1	ASP 1 626	-10.848	-7.855	7.156	1.00	3.31
ATOM	831	OD2	ASP 1 626	-10.199	-6.858	9.037	1.00	3.31
ATOM	832	N	LEU 1 627	-5.704	-8.921	8.184	1.00	5.46

189/208

ATOM	833	CA	LEU	1	627	-4.737	-9.984	8.288	1.00	5.46
ATOM	834	C	LEU	1	627	-3.336	-9.532	8.542	1.00	5.46
ATOM	835	O	LEU	1	627	-2.848	-8.558	7.972	1.00	5.46
ATOM	836	CB	LEU	1	627	-4.741	-10.955	7.086	1.00	5.46
ATOM	837	CG	LEU	1	627	-4.364	-10.353	5.716	1.00	5.46
ATOM	838	CD1	LEU	1	627	-2.877	-9.976	5.633	1.00	5.46
ATOM	839	CD2	LEU	1	627	-4.785	-11.295	4.576	1.00	5.46
ATOM	840	N	ILE	1	628	-2.646	-10.255	9.447	1.00	3.87
ATOM	841	CA	ILE	1	628	-1.294	-9.909	9.743	1.00	3.87
ATOM	842	C	ILE	1	628	-0.443	-10.972	9.139	1.00	3.87
ATOM	843	O	ILE	1	628	-0.757	-12.158	9.228	1.00	3.87
ATOM	844	CB	ILE	1	628	-0.993	-9.828	11.209	1.00	3.87
ATOM	845	CG1	ILE	1	628	0.352	-9.122	11.429	1.00	3.87
ATOM	846	CG2	ILE	1	628	-1.070	-11.245	11.799	1.00	3.87
ATOM	847	CD1	ILE	1	628	0.558	-8.654	12.866	1.00	3.87
ATOM	848	N	ILE	1	629	0.654	-10.561	8.479	1.00	7.73
ATOM	849	CA	ILE	1	629	1.481	-11.529	7.822	1.00	7.73
ATOM	850	C	ILE	1	629	2.901	-11.255	8.179	1.00	7.73
ATOM	851	O	ILE	1	629	3.262	-10.131	8.521	1.00	7.73
ATOM	852	CB	ILE	1	629	1.408	-11.466	6.322	1.00	7.73
ATOM	853	CG1	ILE	1	629	1.985	-10.137	5.798	1.00	7.73
ATOM	854	CG2	ILE	1	629	-0.054	-11.708	5.914	1.00	7.73
ATOM	855	CD1	ILE	1	629	1.253	-8.890	6.291	1.00	7.73
ATOM	856	N	ASN	1	630	3.742	-12.304	8.121	1.00	3.80
ATOM	857	CA	ASN	1	630	5.137	-12.184	8.419	1.00	3.80
ATOM	858	C	ASN	1	630	5.869	-11.907	7.147	1.00	3.80
ATOM	859	O	ASN	1	630	5.289	-11.908	6.062	1.00	3.80
ATOM	860	CB	ASN	1	630	5.738	-13.461	9.031	1.00	3.80
ATOM	861	CG	ASN	1	630	5.595	-14.578	8.007	1.00	3.80
ATOM	862	OD1	ASN	1	630	4.673	-14.573	7.192	1.00	3.80
ATOM	863	ND2	ASN	1	630	6.526	-15.567	8.050	1.00	3.80
ATOM	864	N	GLU	1	631	7.187	-11.662	7.263	1.00	3.57
ATOM	865	CA	GLU	1	631	7.988	-11.375	6.109	1.00	3.57
ATOM	866	C	GLU	1	631	7.926	-12.536	5.169	1.00	3.57
ATOM	867	O	GLU	1	631	7.764	-12.366	3.961	1.00	3.57
ATOM	868	CB	GLU	1	631	9.475	-11.173	6.450	1.00	3.57
ATOM	869	CG	GLU	1	631	10.345	-10.866	5.228	1.00	3.57
ATOM	870	CD	GLU	1	631	11.786	-10.712	5.696	1.00	3.57
ATOM	871	OE1	GLU	1	631	12.099	-9.663	6.319	1.00	3.57
ATOM	872	OE2	GLU	1	631	12.594	-11.644	5.436	1.00	3.57
ATOM	873	N	GLN	1	632	8.037	-13.761	5.707	1.00	5.74
ATOM	874	CA	GLN	1	632	8.056	-14.926	4.874	1.00	5.74
ATOM	875	C	GLN	1	632	6.771	-15.100	4.112	1.00	5.74
ATOM	876	O	GLN	1	632	6.799	-15.379	2.915	1.00	5.74
ATOM	877	CB	GLN	1	632	8.307	-16.215	5.684	1.00	5.74
ATOM	878	CG	GLN	1	632	8.337	-17.501	4.853	1.00	5.74
ATOM	879	CD	GLN	1	632	6.906	-17.987	4.659	1.00	5.74
ATOM	880	OE1	GLN	1	632	6.206	-18.306	5.619	1.00	5.74
ATOM	881	NE2	GLN	1	632	6.451	-18.027	3.378	1.00	5.74
ATOM	882	N	ARG	1	633	5.604	-14.942	4.770	1.00	6.29
ATOM	883	CA	ARG	1	633	4.389	-15.210	4.043	1.00	6.29
ATOM	884	C	ARG	1	633	4.211	-14.188	2.992	1.00	6.29
ATOM	885	O	ARG	1	633	3.685	-14.524	1.937	1.00	6.29
ATOM	886	CB	ARG	1	633	3.055	-15.288	4.868	1.00	6.29
ATOM	887	CG	ARG	1	633	1.781	-15.671	4.039	1.00	6.29
ATOM	888	CD	ARG	1	633	0.503	-16.120	4.825	1.00	6.29
ATOM	889	NE	ARG	1	633	-0.537	-16.684	3.894	1.00	6.29
ATOM	890	CZ	ARG	1	633	-1.381	-17.769	3.971	1.00	6.29
ATOM	891	NH1	ARG	1	633	-1.669	-18.475	5.103	1.00	6.29
ATOM	892	NH2	ARG	1	633	-2.050	-18.131	2.839	1.00	6.29
ATOM	893	N	MET	1	634	4.592	-12.927	3.267	1.00	5.30

190/208

ATOM	894	CA	MET	1 634	4.490	-11.824	2.355	1.00	5.30
ATOM	895	C	MET	1 634	5.504	-11.870	1.253	1.00	5.30
ATOM	896	O	MET	1 634	5.243	-11.342	0.176	1.00	5.30
ATOM	897	CB	MET	1 634	4.655	-10.467	3.043	1.00	5.30
ATOM	898	CG	MET	1 634	6.088	-10.242	3.497	1.00	5.30
ATOM	899	SD	MET	1 634	6.423	-8.596	4.165	1.00	5.30
ATOM	900	CE	MET	1 634	8.197	-8.946	4.143	1.00	5.30
ATOM	901	N	THR	1 635	6.704	-12.449	1.496	1.00	5.56
ATOM	902	CA	THR	1 635	7.691	-12.574	0.448	1.00	5.56
ATOM	903	C	THR	1 635	7.291	-13.593	-0.573	1.00	5.56
ATOM	904	O	THR	1 635	7.247	-13.321	-1.770	1.00	5.56
ATOM	905	CB	THR	1 635	9.057	-12.970	0.948	1.00	5.56
ATOM	906	OG1	THR	1 635	9.976	-13.019	-0.133	1.00	5.56
ATOM	907	CG2	THR	1 635	9.006	-14.304	1.693	1.00	5.56
ATOM	908	N	LEU	1 636	6.921	-14.809	-0.133	1.00	4.24
ATOM	909	CA	LEU	1 636	6.544	-15.813	-1.089	1.00	4.24
ATOM	910	C	LEU	1 636	5.264	-15.595	-1.893	1.00	4.24
ATOM	911	O	LEU	1 636	5.255	-16.010	-3.054	1.00	4.24
ATOM	912	CB	LEU	1 636	6.419	-17.222	-0.478	1.00	4.24
ATOM	913	CG	LEU	1 636	7.748	-17.820	0.028	1.00	4.24
ATOM	914	CD1	LEU	1 636	8.241	-17.113	1.295	1.00	4.24
ATOM	915	CD2	LEU	1 636	7.656	-19.343	0.208	1.00	4.24
ATOM	916	N	PRO	1 637	4.186	-15.012	-1.382	1.00	3.86
ATOM	917	CA	PRO	1 637	2.948	-14.924	-2.088	1.00	3.86
ATOM	918	C	PRO	1 637	3.115	-14.366	-3.410	1.00	3.86
ATOM	919	O	PRO	1 637	2.533	-14.923	-4.330	1.00	3.86
ATOM	920	CB	PRO	1 637	2.043	-14.013	-1.293	1.00	3.86
ATOM	921	CG	PRO	1 637	3.014	-12.991	-0.736	1.00	3.86
ATOM	922	CD	PRO	1 637	4.304	-13.807	-0.651	1.00	3.86
ATOM	923	N	CYS	1 638	3.829	-13.241	-3.498	1.00	3.09
ATOM	924	CA	CYS	1 638	4.111	-12.683	-4.764	1.00	3.09
ATOM	925	C	CYS	1 638	5.156	-11.654	-4.537	1.00	3.09
ATOM	926	O	CYS	1 638	6.022	-11.460	-5.376	1.00	3.09
ATOM	927	CB	CYS	1 638	2.939	-11.903	-5.397	1.00	3.09
ATOM	928	SG	CYS	1 638	1.629	-12.922	-6.146	1.00	3.09
ATOM	929	N	MET	1 639	5.197	-11.038	-3.350	1.00	6.02
ATOM	930	CA	MET	1 639	6.036	-9.884	-3.188	1.00	6.02
ATOM	931	C	MET	1 639	7.487	-10.110	-3.503	1.00	6.02
ATOM	932	O	MET	1 639	8.080	-9.347	-4.263	1.00	6.02
ATOM	933	CB	MET	1 639	5.971	-9.336	-1.753	1.00	6.02
ATOM	934	CG	MET	1 639	4.557	-8.953	-1.308	1.00	6.02
ATOM	935	SD	MET	1 639	3.806	-7.570	-2.217	1.00	6.02
ATOM	936	CE	MET	1 639	2.242	-7.588	-1.297	1.00	6.02
ATOM	937	N	TYR	1 640	8.110	-11.154	-2.931	1.00	5.37
ATOM	938	CA	TYR	1 640	9.491	-11.430	-3.201	1.00	5.37
ATOM	939	C	TYR	1 640	10.263	-10.413	-2.419	1.00	5.37
ATOM	940	O	TYR	1 640	9.991	-10.188	-1.245	1.00	5.37
ATOM	941	CB	TYR	1 640	9.826	-11.396	-4.717	1.00	5.37
ATOM	942	CG	TYR	1 640	11.224	-11.840	-5.002	1.00	5.37
ATOM	943	CD1	TYR	1 640	12.204	-10.952	-5.390	1.00	5.37
ATOM	944	CD2	TYR	1 640	11.555	-13.171	-4.890	1.00	5.37
ATOM	945	CE1	TYR	1 640	13.483	-11.373	-5.655	1.00	5.37
ATOM	946	CE2	TYR	1 640	12.830	-13.603	-5.162	1.00	5.37
ATOM	947	CZ	TYR	1 640	13.797	-12.705	-5.546	1.00	5.37
ATOM	948	OH	TYR	1 640	15.105	-13.146	-5.831	1.00	5.37
ATOM	949	N	ASP	1 641	11.239	-9.752	-3.053	1.00	4.19
ATOM	950	CA	ASP	1 641	12.078	-8.786	-2.414	1.00	4.19
ATOM	951	C	ASP	1 641	11.284	-7.584	-2.016	1.00	4.19
ATOM	952	O	ASP	1 641	11.648	-6.875	-1.080	1.00	4.19
ATOM	953	CB	ASP	1 641	13.244	-8.321	-3.306	1.00	4.19
ATOM	954	CG	ASP	1 641	12.688	-7.658	-4.559	1.00	4.19



191/208

ATOM	955	OD1 ASP 1 641	11.502	-7.911	-4.902	1.00	4.19
ATOM	956	OD2 ASP 1 641	13.457	-6.891	-5.196	1.00	4.19
ATOM	957	N GLN 1 642	10.173	-7.320	-2.723	1.00	3.89
ATOM	958	CA GLN 1 642	9.398	-6.150	-2.438	1.00	3.89
ATOM	959	C GLN 1 642	8.913	-6.211	-1.024	1.00	3.89
ATOM	960	O GLN 1 642	8.788	-5.182	-0.361	1.00	3.89
ATOM	961	CB GLN 1 642	8.180	-5.965	-3.361	1.00	3.89
ATOM	962	CG GLN 1 642	7.354	-4.712	-3.086	1.00	3.89
ATOM	963	CD GLN 1 642	6.027	-4.871	-3.815	1.00	3.89
ATOM	964	OE1 GLN 1 642	5.823	-4.303	-4.883	1.00	3.89
ATOM	965	NE2 GLN 1 642	5.097	-5.669	-3.220	1.00	3.89
ATOM	966	N CYS 1 643	8.626	-7.425	-0.521	1.00	3.75
ATOM	967	CA CYS 1 643	8.132	-7.555	0.820	1.00	3.75
ATOM	968	C CYS 1 643	9.163	-7.043	1.775	1.00	3.75
ATOM	969	O CYS 1 643	8.832	-6.384	2.760	1.00	3.75
ATOM	970	CB CYS 1 643	7.811	-9.006	1.219	1.00	3.75
ATOM	971	SG CYS 1 643	9.300	-10.002	1.508	1.00	3.75
ATOM	972	N LYS 1 644	10.451	-7.320	1.500	1.00	8.40
ATOM	973	CA LYS 1 644	11.497	-6.922	2.387	1.00	8.40
ATOM	974	C LYS 1 644	11.477	-5.434	2.423	1.00	8.40
ATOM	975	O LYS 1 644	11.625	-4.826	3.481	1.00	8.40
ATOM	976	CB LYS 1 644	12.884	-7.374	1.899	1.00	8.40
ATOM	977	CG LYS 1 644	13.980	-7.257	2.959	1.00	8.40
ATOM	978	CD LYS 1 644	13.803	-8.232	4.126	1.00	8.40
ATOM	979	CE LYS 1 644	13.697	-9.696	3.689	1.00	8.40
ATOM	980	NZ LYS 1 644	15.006	-10.177	3.191	1.00	8.40
ATOM	981	N HIS 1 645	11.256	-4.811	1.251	1.00	2.06
ATOM	982	CA HIS 1 645	11.262	-3.382	1.157	1.00	2.06
ATOM	983	C HIS 1 645	10.183	-2.804	2.017	1.00	2.06
ATOM	984	O HIS 1 645	10.409	-1.832	2.734	1.00	2.06
ATOM	985	CB HIS 1 645	11.040	-2.882	-0.279	1.00	2.06
ATOM	986	CG HIS 1 645	11.300	-1.414	-0.432	1.00	2.06
ATOM	987	ND1 HIS 1 645	11.608	-0.808	-1.630	1.00	2.06
ATOM	988	CD2 HIS 1 645	11.279	-0.416	0.493	1.00	2.06
ATOM	989	CE1 HIS 1 645	11.762	0.515	-1.371	1.00	2.06
ATOM	990	NE2 HIS 1 645	11.572	0.801	-0.096	1.00	2.06
ATOM	991	N MET 1 646	8.976	-3.394	1.970	1.00	2.52
ATOM	992	CA MET 1 646	7.880	-2.894	2.749	1.00	2.52
ATOM	993	C MET 1 646	8.163	-3.056	4.213	1.00	2.52
ATOM	994	O MET 1 646	7.864	-2.167	5.008	1.00	2.52
ATOM	995	CB MET 1 646	6.557	-3.626	2.455	1.00	2.52
ATOM	996	CG MET 1 646	6.032	-3.396	1.036	1.00	2.52
ATOM	997	SD MET 1 646	4.470	-4.249	0.661	1.00	2.52
ATOM	998	CE MET 1 646	4.358	-3.638	-1.046	1.00	2.52
ATOM	999	N LEU 1 647	8.741	-4.200	4.623	1.00	1.01
ATOM	1000	CA LEU 1 647	8.998	-4.389	6.025	1.00	1.01
ATOM	1001	C LEU 1 647	9.958	-3.366	6.506	1.00	1.01
ATOM	1002	O LEU 1 647	9.743	-2.749	7.548	1.00	1.01
ATOM	1003	CB LEU 1 647	9.690	-5.708	6.383	1.00	1.01
ATOM	1004	CG LEU 1 647	8.838	-6.958	6.180	1.00	1.01
ATOM	1005	CD1 LEU 1 647	9.605	-8.211	6.620	1.00	1.01
ATOM	1006	CD2 LEU 1 647	7.461	-6.831	6.834	1.00	1.01
ATOM	1007	N TYR 1 648	11.063	-3.160	5.767	1.00	6.90
ATOM	1008	CA TYR 1 648	11.990	-2.202	6.272	1.00	6.90
ATOM	1009	C TYR 1 648	11.426	-0.823	6.265	1.00	6.90
ATOM	1010	O TYR 1 648	11.736	-0.029	7.153	1.00	6.90
ATOM	1011	CB TYR 1 648	13.429	-2.259	5.705	1.00	6.90
ATOM	1012	CG TYR 1 648	13.499	-2.469	4.232	1.00	6.90
ATOM	1013	CD1 TYR 1 648	13.274	-1.450	3.336	1.00	6.90
ATOM	1014	CD2 TYR 1 648	14.075	-3.633	3.776	1.00	6.90
ATOM	1015	CE1 TYR 1 648	13.566	-1.623	2.002	1.00	6.90

192/208

ATOM	1016	CE2 TYR 1 648	14.368	-3.814	2.447	1.00	6.90
ATOM	1017	CZ TYR 1 648	14.122	-2.800	1.556	1.00	6.90
ATOM	1018	OH TYR 1 648	14.436	-2.970	0.191	1.00	6.90
ATOM	1019	N VAL 1 649	10.571	-0.484	5.282	1.00	3.24
ATOM	1020	CA VAL 1 649	10.016	0.835	5.329	1.00	3.24
ATOM	1021	C VAL 1 649	9.185	0.944	6.569	1.00	3.24
ATOM	1022	O VAL 1 649	9.226	1.955	7.268	1.00	3.24
ATOM	1023	CB VAL 1 649	9.165	1.206	4.143	1.00	3.24
ATOM	1024	CG1 VAL 1 649	7.840	0.434	4.182	1.00	3.24
ATOM	1025	CG2 VAL 1 649	8.973	2.732	4.155	1.00	3.24
ATOM	1026	N SER 1 650	8.423	-0.116	6.895	1.00	3.01
ATOM	1027	CA SER 1 650	7.588	-0.062	8.057	1.00	3.01
ATOM	1028	C SER 1 650	8.382	0.080	9.315	1.00	3.01
ATOM	1029	O SER 1 650	7.972	0.789	10.232	1.00	3.01
ATOM	1030	CB SER 1 650	6.728	-1.292	8.289	1.00	3.01
ATOM	1031	OG SER 1 650	6.141	-1.100	9.562	1.00	3.01
ATOM	1032	N SER 1 651	9.529	-0.615	9.408	1.00	3.21
ATOM	1033	CA SER 1 651	10.305	-0.555	10.611	1.00	3.21
ATOM	1034	C SER 1 651	10.788	0.846	10.809	1.00	3.21
ATOM	1035	O SER 1 651	10.753	1.373	11.919	1.00	3.21
ATOM	1036	CB SER 1 651	11.543	-1.467	10.566	1.00	3.21
ATOM	1037	OG SER 1 651	12.442	-1.019	9.562	1.00	3.21
ATOM	1038	N GLU 1 652	11.247	1.482	9.715	1.00	3.30
ATOM	1039	CA GLU 1 652	11.786	2.811	9.744	1.00	3.30
ATOM	1040	C GLU 1 652	10.741	3.828	10.087	1.00	3.30
ATOM	1041	O GLU 1 652	11.018	4.810	10.772	1.00	3.30
ATOM	1042	CB GLU 1 652	12.417	3.215	8.399	1.00	3.30
ATOM	1043	CG GLU 1 652	13.164	4.548	8.446	1.00	3.30
ATOM	1044	CD GLU 1 652	13.852	4.745	7.102	1.00	3.30
ATOM	1045	OE1 GLU 1 652	14.492	3.772	6.620	1.00	3.30
ATOM	1046	OE2 GLU 1 652	13.746	5.866	6.538	1.00	3.30
ATOM	1047	N LEU 1 653	9.502	3.601	9.613	1.00	1.22
ATOM	1048	CA LEU 1 653	8.382	4.490	9.772	1.00	1.22
ATOM	1049	C LEU 1 653	7.999	4.675	11.205	1.00	1.22
ATOM	1050	O LEU 1 653	7.473	5.722	11.576	1.00	1.22
ATOM	1051	CB LEU 1 653	7.121	3.976	9.055	1.00	1.22
ATOM	1052	CG LEU 1 653	7.274	3.871	7.529	1.00	1.22
ATOM	1053	CD1 LEU 1 653	5.985	3.356	6.869	1.00	1.22
ATOM	1054	CD2 LEU 1 653	7.759	5.198	6.931	1.00	1.22
ATOM	1055	N HIS 1 654	8.239	3.664	12.056	1.00	0.94
ATOM	1056	CA HIS 1 654	7.780	3.733	13.412	1.00	0.94
ATOM	1057	C HIS 1 654	8.305	4.961	14.097	1.00	0.94
ATOM	1058	O HIS 1 654	7.566	5.632	14.816	1.00	0.94
ATOM	1059	CB HIS 1 654	8.210	2.509	14.238	1.00	0.94
ATOM	1060	CG HIS 1 654	7.684	1.227	13.664	1.00	0.94
ATOM	1061	ND1 HIS 1 654	6.369	0.824	13.747	1.00	0.94
ATOM	1062	CD2 HIS 1 654	8.323	0.263	12.946	1.00	0.94
ATOM	1063	CE1 HIS 1 654	6.279	-0.354	13.078	1.00	0.94
ATOM	1064	NE2 HIS 1 654	7.440	-0.735	12.578	1.00	0.94
ATOM	1065	N ARG 1 655	9.588	5.300	13.882	1.00	4.48
ATOM	1066	CA ARG 1 655	10.187	6.440	14.522	1.00	4.48
ATOM	1067	C ARG 1 655	9.540	7.715	14.072	1.00	4.48
ATOM	1068	O ARG 1 655	9.425	8.669	14.840	1.00	4.48
ATOM	1069	CB ARG 1 655	11.691	6.574	14.233	1.00	4.48
ATOM	1070	CG ARG 1 655	12.538	5.463	14.856	1.00	4.48
ATOM	1071	CD ARG 1 655	14.043	5.712	14.741	1.00	4.48
ATOM	1072	NE ARG 1 655	14.368	6.866	15.627	1.00	4.48
ATOM	1073	CZ ARG 1 655	15.669	7.202	15.868	1.00	4.48
ATOM	1074	NH1 ARG 1 655	15.961	8.258	16.682	1.00	4.48
ATOM	1075	NH2 ARG 1 655	16.677	6.484	15.293	1.00	4.48
ATOM	1076	N LEU 1 656	9.101	7.757	12.802	1.00	6.60

193/208

ATOM 1077 CA LEU 1 656	8.539	8.936	12.207	1.00	6.60
ATOM 1078 C LEU 1 656	7.300	9.335	12.952	1.00	6.60
ATOM 1079 O LEU 1 656	6.991	10.521	13.063	1.00	6.60
ATOM 1080 CB LEU 1 656	8.207	8.718	10.718	1.00	6.60
ATOM 1081 CG LEU 1 656	7.801	9.993	9.959	1.00	6.60
ATOM 1082 CD1 LEU 1 656	8.927	11.038	9.999	1.00	6.60
ATOM 1083 CD2 LEU 1 656	7.394	9.665	8.514	1.00	6.60
ATOM 1084 N GLN 1 657	6.552	8.349	13.484	1.00	4.61
ATOM 1085 CA GLN 1 657	5.373	8.650	14.248	1.00	4.61
ATOM 1086 C GLN 1 657	4.426	9.452	13.422	1.00	4.61
ATOM 1087 O GLN 1 657	4.006	10.537	13.822	1.00	4.61
ATOM 1088 CB GLN 1 657	5.670	9.464	15.521	1.00	4.61
ATOM 1089 CG GLN 1 657	6.537	8.726	16.543	1.00	4.61
ATOM 1090 CD GLN 1 657	5.673	7.683	17.234	1.00	4.61
ATOM 1091 OE1 GLN 1 657	6.155	6.910	18.062	1.00	4.61
ATOM 1092 NE2 GLN 1 657	4.358	7.659	16.892	1.00	4.61
ATOM 1093 N VAL 1 658	4.057	8.932	12.237	1.00	4.09
ATOM 1094 CA VAL 1 658	3.151	9.662	11.405	1.00	4.09
ATOM 1095 C VAL 1 658	1.751	9.432	11.857	1.00	4.09
ATOM 1096 O VAL 1 658	1.415	8.383	12.406	1.00	4.09
ATOM 1097 CB VAL 1 658	3.196	9.282	9.954	1.00	4.09
ATOM 1098 CG1 VAL 1 658	4.593	9.604	9.412	1.00	4.09
ATOM 1099 CG2 VAL 1 658	2.781	7.811	9.803	1.00	4.09
ATOM 1100 N SER 1 659	0.893	10.447	11.648	1.00	5.48
ATOM 1101 CA SER 1 659	-0.487	10.313	11.998	1.00	5.48
ATOM 1102 C SER 1 659	-1.244	10.189	10.719	1.00	5.48
ATOM 1103 O SER 1 659	-0.664	10.146	9.635	1.00	5.48
ATOM 1104 CB SER 1 659	-1.056	11.510	12.768	1.00	5.48
ATOM 1105 OG SER 1 659	-0.398	11.640	14.020	1.00	5.48
ATOM 1106 N TYR 1 660	-2.582	10.134	10.816	1.00	4.14
ATOM 1107 CA TYR 1 660	-3.380	9.977	9.642	1.00	4.14
ATOM 1108 C TYR 1 660	-3.203	11.111	8.680	1.00	4.14
ATOM 1109 O TYR 1 660	-3.173	10.886	7.474	1.00	4.14
ATOM 1110 CB TYR 1 660	-4.869	9.731	9.952	1.00	4.14
ATOM 1111 CG TYR 1 660	-5.313	10.667	11.021	1.00	4.14
ATOM 1112 CD1 TYR 1 660	-4.992	10.401	12.333	1.00	4.14
ATOM 1113 CD2 TYR 1 660	-6.192	11.686	10.751	1.00	4.14
ATOM 1114 CE1 TYR 1 660	-5.513	11.159	13.354	1.00	4.14
ATOM 1115 CE2 TYR 1 660	-6.718	12.451	11.766	1.00	4.14
ATOM 1116 CZ TYR 1 660	-6.383	12.184	13.071	1.00	4.14
ATOM 1117 OH TYR 1 660	-6.940	12.949	14.117	1.00	4.14
ATOM 1118 N GLU 1 661	-3.055	12.357	9.166	1.00	3.59
ATOM 1119 CA GLU 1 661	-2.906	13.461	8.257	1.00	3.59
ATOM 1120 C GLU 1 661	-1.654	13.326	7.442	1.00	3.59
ATOM 1121 O GLU 1 661	-1.658	13.567	6.235	1.00	3.59
ATOM 1122 CB GLU 1 661	-2.847	14.820	8.973	1.00	3.59
ATOM 1123 CG GLU 1 661	-1.677	14.957	9.948	1.00	3.59
ATOM 1124 CD GLU 1 661	-1.767	16.345	10.567	1.00	3.59
ATOM 1125 OE1 GLU 1 661	-1.886	17.329	9.790	1.00	3.59
ATOM 1126 OE2 GLU 1 661	-1.728	16.440	11.822	1.00	3.59
ATOM 1127 N GLU 1 662	-0.542	12.935	8.085	1.00	1.15
ATOM 1128 CA GLU 1 662	0.708	12.809	7.393	1.00	1.15
ATOM 1129 C GLU 1 662	0.611	11.716	6.372	1.00	1.15
ATOM 1130 O GLU 1 662	1.114	11.856	5.259	1.00	1.15
ATOM 1131 CB GLU 1 662	1.866	12.534	8.369	1.00	1.15
ATOM 1132 CG GLU 1 662	2.138	13.747	9.268	1.00	1.15
ATOM 1133 CD GLU 1 662	3.040	13.341	10.425	1.00	1.15
ATOM 1134 OE1 GLU 1 662	2.691	12.356	11.130	1.00	1.15
ATOM 1135 OE2 GLU 1 662	4.085	14.016	10.624	1.00	1.15
ATOM 1136 N TYR 1 663	-0.048	10.591	6.720	1.00	6.52
ATOM 1137 CA TYR 1 663	-0.196	9.526	5.767	1.00	6.52

SUBSTITUTE SHEET (RULE 26)

194/208

ATOM 1138 C TYR 1 663	-1.042	9.982	4.620	1.00	6.52
ATOM 1139 O TYR 1 663	-0.767	9.640	3.472	1.00	6.52
ATOM 1140 CB TYR 1 663	-0.819	8.241	6.339	1.00	6.52
ATOM 1141 CG TYR 1 663	-1.054	7.337	5.175	1.00	6.52
ATOM 1142 CD1 TYR 1 663	-0.005	6.939	4.378	1.00	6.52
ATOM 1143 CD2 TYR 1 663	-2.288	6.761	4.971	1.00	6.52
ATOM 1144 CE1 TYR 1 663	-0.205	6.071	3.331	1.00	6.52
ATOM 1145 CE2 TYR 1 663	-2.484	5.855	3.955	1.00	6.52
ATOM 1146 CZ TYR 1 663	-1.445	5.526	3.115	1.00	6.52
ATOM 1147 OH TYR 1 663	-1.644	4.624	2.049	1.00	6.52
ATOM 1148 N LEU 1 664	-2.101	10.772	4.896	1.00	4.94
ATOM 1149 CA LEU 1 664	-2.936	11.261	3.833	1.00	4.94
ATOM 1150 C LEU 1 664	-2.160	12.062	2.863	1.00	4.94
ATOM 1151 O LEU 1 664	-2.253	11.872	1.652	1.00	4.94
ATOM 1152 CB LEU 1 664	-3.980	12.302	4.252	1.00	4.94
ATOM 1153 CG LEU 1 664	-5.336	11.712	4.558	1.00	4.94
ATOM 1154 CD1 LEU 1 664	-5.727	10.909	3.315	1.00	4.94
ATOM 1155 CD2 LEU 1 664	-5.408	11.006	5.915	1.00	4.94
ATOM 1156 N CYS 1 665	-1.380	12.996	3.409	1.00	0.94
ATOM 1157 CA CYS 1 665	-0.635	13.934	2.643	1.00	0.94
ATOM 1158 C CYS 1 665	0.294	13.182	1.757	1.00	0.94
ATOM 1159 O CYS 1 665	0.441	13.492	0.576	1.00	0.94
ATOM 1160 CB CYS 1 665	0.222	14.789	3.581	1.00	0.94
ATOM 1161 SG CYS 1 665	-0.788	15.819	4.692	1.00	0.94
ATOM 1162 N MET 1 666	0.948	12.155	2.317	1.00	4.36
ATOM 1163 CA MET 1 666	1.880	11.401	1.544	1.00	4.36
ATOM 1164 C MET 1 666	1.150	10.699	0.442	1.00	4.36
ATOM 1165 O MET 1 666	1.642	10.625	-0.683	1.00	4.36
ATOM 1166 CB MET 1 666	2.668	10.379	2.382	1.00	4.36
ATOM 1167 CG MET 1 666	1.864	9.172	2.858	1.00	4.36
ATOM 1168 SD MET 1 666	2.829	8.023	3.882	1.00	4.36
ATOM 1169 CE MET 1 666	4.183	7.920	2.678	1.00	4.36
ATOM 1170 N LYS 1 667	-0.059	10.178	0.729	1.00	2.57
ATOM 1171 CA LYS 1 667	-0.804	9.480	-0.281	1.00	2.57
ATOM 1172 C LYS 1 667	-1.119	10.417	-1.402	1.00	2.57
ATOM 1173 O LYS 1 667	-1.000	10.056	-2.572	1.00	2.57
ATOM 1174 CB LYS 1 667	-2.168	8.953	0.189	1.00	2.57
ATOM 1175 CG LYS 1 667	-2.117	7.815	1.204	1.00	2.57
ATOM 1176 CD LYS 1 667	-3.513	7.385	1.660	1.00	2.57
ATOM 1177 CE LYS 1 667	-4.251	6.536	0.622	1.00	2.57
ATOM 1178 NZ LYS 1 667	-5.555	6.092	1.163	1.00	2.57
ATOM 1179 N THR 1 668	-1.533	11.654	-1.069	1.00	5.21
ATOM 1180 CA THR 1 668	-1.916	12.584	-2.089	1.00	5.21
ATOM 1181 C THR 1 668	-0.743	12.889	-2.960	1.00	5.21
ATOM 1182 O THR 1 668	-0.876	12.992	-4.177	1.00	5.21
ATOM 1183 CB THR 1 668	-2.435	13.893	-1.555	1.00	5.21
ATOM 1184 OG1 THR 1 668	-1.418	14.575	-0.837	1.00	5.21
ATOM 1185 CG2 THR 1 668	-3.633	13.612	-0.634	1.00	5.21
ATOM 1186 N LEU 1 669	0.456	13.042	-2.378	1.00	0.92
ATOM 1187 CA LEU 1 669	1.555	13.381	-3.230	1.00	0.92
ATOM 1188 C LEU 1 669	1.838	12.252	-4.172	1.00	0.92
ATOM 1189 O LEU 1 669	2.136	12.473	-5.344	1.00	0.92
ATOM 1190 CB LEU 1 669	2.847	13.743	-2.480	1.00	0.92
ATOM 1191 CG LEU 1 669	3.977	14.146	-3.444	1.00	0.92
ATOM 1192 CD1 LEU 1 669	3.543	15.317	-4.339	1.00	0.92
ATOM 1193 CD2 LEU 1 669	5.270	14.473	-2.686	1.00	0.92
ATOM 1194 N LEU 1 670	1.738	11.000	-3.686	1.00	0.69
ATOM 1195 CA LEU 1 670	2.018	9.865	-4.520	1.00	0.69
ATOM 1196 C LEU 1 670	1.049	9.837	-5.661	1.00	0.69
ATOM 1197 O LEU 1 670	1.430	9.611	-6.810	1.00	0.69
ATOM 1198 CB LEU 1 670	1.861	8.535	-3.763	1.00	0.69

195/208

ATOM 1199	CG LEU 1 670	2.854	8.365	-2.599	1.00	0.69
ATOM 1200	CD1 LEU 1 670	2.651	7.018	-1.890	1.00	0.69
ATOM 1201	CD2 LEU 1 670	4.305	8.572	-3.066	1.00	0.69
ATOM 1202	N LEU 1 671	-0.240	10.082	-5.368	1.00	3.54
ATOM 1203	CA LEU 1 671	-1.272	10.024	-6.364	1.00	3.54
ATOM 1204	C LEU 1 671	-1.070	11.102	-7.383	1.00	3.54
ATOM 1205	O LEU 1 671	-1.261	10.883	-8.577	1.00	3.54
ATOM 1206	CB LEU 1 671	-2.678	10.108	-5.728	1.00	3.54
ATOM 1207	CG LEU 1 671	-3.861	10.063	-6.716	1.00	3.54
ATOM 1208	CD1 LEU 1 671	-5.177	9.741	-5.994	1.00	3.54
ATOM 1209	CD2 LEU 1 671	-3.993	11.377	-7.493	1.00	3.54
ATOM 1210	N LEU 1 672	-0.642	12.284	-6.918	1.00	5.01
ATOM 1211	CA LEU 1 672	-0.396	13.478	-7.671	1.00	5.01
ATOM 1212	C LEU 1 672	0.765	13.403	-8.606	1.00	5.01
ATOM 1213	O LEU 1 672	1.018	14.367	-9.325	1.00	5.01
ATOM 1214	CB LEU 1 672	-0.250	14.727	-6.797	1.00	5.01
ATOM 1215	CG LEU 1 672	-1.602	15.358	-6.418	1.00	5.01
ATOM 1216	CD1 LEU 1 672	-2.591	14.356	-5.807	1.00	5.01
ATOM 1217	CD2 LEU 1 672	-1.363	16.565	-5.508	1.00	5.01
ATOM 1218	N SER 1 673	1.564	12.322	-8.549	1.00	4.46
ATOM 1219	CA SER 1 673	2.677	12.205	-9.450	1.00	4.46
ATOM 1220	C SER 1 673	2.229	12.452	-10.854	1.00	4.46
ATOM 1221	O SER 1 673	1.485	11.670	-11.444	1.00	4.46
ATOM 1222	CB SER 1 673	3.371	10.834	-9.381	1.00	4.46
ATOM 1223	OG SER 1 673	2.450	9.808	-9.715	1.00	4.46
ATOM 1224	N SER 1 674	2.710	13.573	-11.422	1.00	4.03
ATOM 1225	CA SER 1 674	2.324	14.023	-12.726	1.00	4.03
ATOM 1226	C SER 1 674	3.197	13.391	-13.750	1.00	4.03
ATOM 1227	O SER 1 674	2.937	12.281	-14.209	1.00	4.03
ATOM 1228	CB SER 1 674	2.464	15.545	-12.902	1.00	4.03
ATOM 1229	OG SER 1 674	1.589	16.226	-12.016	1.00	4.03
ATOM 1230	N VAL 1 675	4.265	14.110	-14.135	1.00	4.27
ATOM 1231	CA VAL 1 675	5.158	13.662	-15.158	1.00	4.27
ATOM 1232	C VAL 1 675	5.648	12.258	-14.953	1.00	4.27
ATOM 1233	O VAL 1 675	6.039	11.636	-15.940	1.00	4.27
ATOM 1234	CB VAL 1 675	6.348	14.565	-15.353	1.00	4.27
ATOM 1235	CG1 VAL 1 675	7.204	14.599	-14.077	1.00	4.27
ATOM 1236	CG2 VAL 1 675	7.113	14.081	-16.596	1.00	4.27
ATOM 1237	N PRO 1 676	5.668	11.678	-13.779	1.00	2.47
ATOM 1238	CA PRO 1 676	6.142	10.328	-13.718	1.00	2.47
ATOM 1239	C PRO 1 676	5.180	9.425	-14.410	1.00	2.47
ATOM 1240	O PRO 1 676	5.538	8.290	-14.721	1.00	2.47
ATOM 1241	CB PRO 1 676	6.368	10.014	-12.235	1.00	2.47
ATOM 1242	CG PRO 1 676	5.825	11.241	-11.479	1.00	2.47
ATOM 1243	CD PRO 1 676	5.899	12.365	-12.518	1.00	2.47
ATOM 1244	N LYS 1 677	3.953	9.909	-14.647	1.00	7.09
ATOM 1245	CA LYS 1 677	2.953	9.130	-15.305	1.00	7.09
ATOM 1246	C LYS 1 677	3.295	9.075	-16.754	1.00	7.09
ATOM 1247	O LYS 1 677	3.876	10.009	-17.301	1.00	7.09
ATOM 1248	CB LYS 1 677	1.565	9.786	-15.268	1.00	7.09
ATOM 1249	CG LYS 1 677	0.945	9.990	-13.886	1.00	7.09
ATOM 1250	CD LYS 1 677	0.660	8.694	-13.134	1.00	7.09
ATOM 1251	CE LYS 1 677	1.641	8.443	-11.994	1.00	7.09
ATOM 1252	NZ LYS 1 677	3.004	8.241	-12.528	1.00	7.09
ATOM 1253	N ASP 1 678	2.936	7.960	-17.414	1.00	3.66
ATOM 1254	CA ASP 1 678	3.159	7.842	-18.822	1.00	3.66
ATOM 1255	C ASP 1 678	1.804	7.942	-19.448	1.00	3.66
ATOM 1256	O ASP 1 678	0.919	7.138	-19.154	1.00	3.66
ATOM 1257	CB ASP 1 678	3.754	6.479	-19.221	1.00	3.66
ATOM 1258	CG ASP 1 678	4.010	6.465	-20.722	1.00	3.66
ATOM 1259	OD1 ASP 1 678	3.687	7.483	-21.392	1.00	3.66

SUBSTITUTE SHEET (RULE 26)

196/208

ATOM	1260	OD2 ASP 1 678	4.529	5.431	-21.220	1.00	3.66
ATOM	1261	N GLY 1 679	1.600	8.946	-20.323	1.00	0.72
ATOM	1262	CA GLY 1 679	0.337	9.069	-20.992	1.00	0.72
ATOM	1263	C GLY 1 679	-0.557	10.104	-20.372	1.00	0.72
ATOM	1264	O GLY 1 679	-1.593	10.440	-20.942	1.00	0.72
ATOM	1265	N LEU 1 680	-0.195	10.641	-19.189	1.00	3.91
ATOM	1266	CA LEU 1 680	-1.015	11.655	-18.577	1.00	3.91
ATOM	1267	C LEU 1 680	-1.041	12.859	-19.453	1.00	3.91
ATOM	1268	O LEU 1 680	0.005	13.396	-19.817	1.00	3.91
ATOM	1269	CB LEU 1 680	-0.504	12.083	-17.185	1.00	3.91
ATOM	1270	CG LEU 1 680	-0.962	11.201	-16.007	1.00	3.91
ATOM	1271	CD1 LEU 1 680	-2.274	11.711	-15.404	1.00	3.91
ATOM	1272	CD2 LEU 1 680	-1.132	9.738	-16.439	1.00	3.91
ATOM	1273	N LYS 1 681	-2.252	13.279	-19.873	1.00	9.62
ATOM	1274	CA LYS 1 681	-2.324	14.444	-20.700	1.00	9.62
ATOM	1275	C LYS 1 681	-2.135	15.726	-19.952	1.00	9.62
ATOM	1276	O LYS 1 681	-1.432	16.617	-20.426	1.00	9.62
ATOM	1277	CB LYS 1 681	-3.605	14.566	-21.542	1.00	9.62
ATOM	1278	CG LYS 1 681	-4.874	14.922	-20.780	1.00	9.62
ATOM	1279	CD LYS 1 681	-5.342	13.847	-19.810	1.00	9.62
ATOM	1280	CE LYS 1 681	-6.817	14.021	-19.474	1.00	9.62
ATOM	1281	NZ LYS 1 681	-7.616	13.820	-20.704	1.00	9.62
ATOM	1282	N SER 1 682	-2.741	15.867	-18.753	1.00	3.76
ATOM	1283	CA SER 1 682	-2.629	17.141	-18.102	1.00	3.76
ATOM	1284	C SER 1 682	-1.576	17.102	-17.041	1.00	3.76
ATOM	1285	O SER 1 682	-1.874	17.009	-15.851	1.00	3.76
ATOM	1286	CB SER 1 682	-3.935	17.597	-17.438	1.00	3.76
ATOM	1287	OG SER 1 682	-3.752	18.895	-16.898	1.00	3.76
ATOM	1288	N GLN 1 683	-0.300	17.189	-17.456	1.00	3.60
ATOM	1289	CA GLN 1 683	0.774	17.152	-16.511	1.00	3.60
ATOM	1290	C GLN 1 683	0.808	18.390	-15.668	1.00	3.60
ATOM	1291	O GLN 1 683	1.001	18.313	-14.457	1.00	3.60
ATOM	1292	CB GLN 1 683	2.158	17.009	-17.167	1.00	3.60
ATOM	1293	CG GLN 1 683	2.560	18.199	-18.039	1.00	3.60
ATOM	1294	CD GLN 1 683	3.940	17.908	-18.610	1.00	3.60
ATOM	1295	OE1 GLN 1 683	4.530	16.864	-18.336	1.00	3.60
ATOM	1296	NE2 GLN 1 683	4.475	18.857	-19.425	1.00	3.60
ATOM	1297	N GLU 1 684	0.603	19.567	-16.290	1.00	3.13
ATOM	1298	CA GLU 1 684	0.756	20.811	-15.586	1.00	3.13
ATOM	1299	C GLU 1 684	-0.201	21.003	-14.452	1.00	3.13
ATOM	1300	O GLU 1 684	0.216	21.351	-13.349	1.00	3.13
ATOM	1301	CB GLU 1 684	0.622	22.033	-16.511	1.00	3.13
ATOM	1302	CG GLU 1 684	1.772	22.148	-17.513	1.00	3.13
ATOM	1303	CD GLU 1 684	3.054	22.373	-16.723	1.00	3.13
ATOM	1304	OE1 GLU 1 684	2.967	22.482	-15.472	1.00	3.13
ATOM	1305	OE2 GLU 1 684	4.139	22.436	-17.362	1.00	3.13
ATOM	1306	N LEU 1 685	-1.509	20.769	-14.668	1.00	7.18
ATOM	1307	CA LEU 1 685	-2.427	21.022	-13.593	1.00	7.18
ATOM	1308	C LEU 1 685	-2.104	20.082	-12.491	1.00	7.18
ATOM	1309	O LEU 1 685	-2.183	20.414	-11.310	1.00	7.18
ATOM	1310	CB LEU 1 685	-3.919	20.860	-13.977	1.00	7.18
ATOM	1311	CG LEU 1 685	-4.434	19.429	-14.259	1.00	7.18
ATOM	1312	CD1 LEU 1 685	-4.558	18.563	-12.993	1.00	7.18
ATOM	1313	CD2 LEU 1 685	-5.752	19.480	-15.047	1.00	7.18
ATOM	1314	N PHE 1 686	-1.737	18.859	-12.885	1.00	3.83
ATOM	1315	CA PHE 1 686	-1.447	17.791	-11.989	1.00	3.83
ATOM	1316	C PHE 1 686	-0.251	18.129	-11.151	1.00	3.83
ATOM	1317	O PHE 1 686	-0.213	17.840	-9.954	1.00	3.83
ATOM	1318	CB PHE 1 686	-1.208	16.527	-12.809	1.00	3.83
ATOM	1319	CG PHE 1 686	-1.341	15.429	-11.852	1.00	3.83
ATOM	1320	CD1 PHE 1 686	-2.481	15.350	-11.090	1.00	3.83

197/208

ATOM	1321	CD2 PHE 1 686	-0.486	14.369	-11.931	1.00	3.83
ATOM	1322	CE1 PHE 1 686	-2.676	14.293	-10.247	1.00	3.83
ATOM	1323	CE2 PHE 1 686	-0.708	13.282	-11.144	1.00	3.83
ATOM	1324	CZ PHE 1 686	-1.751	13.284	-10.258	1.00	3.83
ATOM	1325	N ASP 1 687	0.768	18.753	-11.768	1.00	4.20
ATOM	1326	CA ASP 1 687	1.949	19.143	-11.056	1.00	4.20
ATOM	1327	C ASP 1 687	1.566	20.206	-10.078	1.00	4.20
ATOM	1328	O ASP 1 687	2.041	20.230	-8.943	1.00	4.20
ATOM	1329	CB ASP 1 687	3.032	19.728	-11.978	1.00	4.20
ATOM	1330	CG ASP 1 687	4.308	19.892	-11.165	1.00	4.20
ATOM	1331	OD1 ASP 1 687	5.331	20.338	-11.752	1.00	4.20
ATOM	1332	OD2 ASP 1 687	4.279	19.570	-9.948	1.00	4.20
ATOM	1333	N GLU 1 688	0.669	21.115	-10.499	1.00	1.12
ATOM	1334	CA GLU 1 688	0.259	22.192	-9.649	1.00	1.12
ATOM	1335	C GLU 1 688	-0.378	21.601	-8.437	1.00	1.12
ATOM	1336	O GLU 1 688	-0.161	22.052	-7.313	1.00	1.12
ATOM	1337	CB GLU 1 688	-0.788	23.103	-10.312	1.00	1.12
ATOM	1338	CG GLU 1 688	-0.249	23.904	-11.497	1.00	1.12
ATOM	1339	CD GLU 1 688	-1.408	24.693	-12.086	1.00	1.12
ATOM	1340	OE1 GLU 1 688	-1.157	25.526	-12.997	1.00	1.12
ATOM	1341	OE2 GLU 1 688	-2.563	24.470	-11.635	1.00	1.12
ATOM	1342	N ILE 1 689	-1.196	20.559	-8.634	1.00	3.95
ATOM	1343	CA ILE 1 689	-1.864	19.967	-7.519	1.00	3.95
ATOM	1344	C ILE 1 689	-0.849	19.371	-6.598	1.00	3.95
ATOM	1345	O ILE 1 689	-0.917	19.555	-5.385	1.00	3.95
ATOM	1346	CB ILE 1 689	-2.812	18.880	-7.932	1.00	3.95
ATOM	1347	CG1 ILE 1 689	-3.859	19.434	-8.913	1.00	3.95
ATOM	1348	CG2 ILE 1 689	-3.448	18.299	-6.659	1.00	3.95
ATOM	1349	CD1 ILE 1 689	-4.718	20.551	-8.321	1.00	3.95
ATOM	1350	N ARG 1 690	0.153	18.658	-7.135	1.00	7.53
ATOM	1351	CA ARG 1 690	1.086	18.025	-6.251	1.00	7.53
ATOM	1352	C ARG 1 690	1.845	19.026	-5.444	1.00	7.53
ATOM	1353	O ARG 1 690	2.016	18.847	-4.239	1.00	7.53
ATOM	1354	CB ARG 1 690	2.112	17.131	-6.970	1.00	7.53
ATOM	1355	CG ARG 1 690	3.021	17.870	-7.953	1.00	7.53
ATOM	1356	CD ARG 1 690	4.037	16.952	-8.632	1.00	7.53
ATOM	1357	NE ARG 1 690	4.936	16.430	-7.564	1.00	7.53
ATOM	1358	CZ ARG 1 690	5.289	15.111	-7.550	1.00	7.53
ATOM	1359	NH1 ARG 1 690	6.109	14.637	-6.566	1.00	7.53
ATOM	1360	NH2 ARG 1 690	4.819	14.267	-8.514	1.00	7.53
ATOM	1361	N MET 1 691	2.310	20.127	-6.064	1.00	8.51
ATOM	1362	CA MET 1 691	3.098	21.007	-5.254	1.00	8.51
ATOM	1363	C MET 1 691	2.254	21.587	-4.169	1.00	8.51
ATOM	1364	O MET 1 691	2.743	21.819	-3.064	1.00	8.51
ATOM	1365	CB MET 1 691	3.846	22.155	-5.971	1.00	8.51
ATOM	1366	CG MET 1 691	3.084	23.466	-6.180	1.00	8.51
ATOM	1367	SD MET 1 691	2.189	23.618	-7.747	1.00	8.51
ATOM	1368	CE MET 1 691	3.673	23.884	-8.758	1.00	8.51
ATOM	1369	N THR 1 692	0.958	21.838	-4.439	1.00	4.62
ATOM	1370	CA THR 1 692	0.168	22.427	-3.398	1.00	4.62
ATOM	1371	C THR 1 692	0.124	21.491	-2.231	1.00	4.62
ATOM	1372	O THR 1 692	0.213	21.924	-1.083	1.00	4.62
ATOM	1373	CB THR 1 692	-1.245	22.771	-3.789	1.00	4.62
ATOM	1374	OG1 THR 1 692	-1.808	23.642	-2.819	1.00	4.62
ATOM	1375	CG2 THR 1 692	-2.094	21.496	-3.868	1.00	4.62
ATOM	1376	N TYR 1 693	-0.014	20.175	-2.487	1.00	1.13
ATOM	1377	CA TYR 1 693	-0.051	19.248	-1.393	1.00	1.13
ATOM	1378	C TYR 1 693	1.261	19.240	-0.685	1.00	1.13
ATOM	1379	O TYR 1 693	1.294	19.257	0.542	1.00	1.13
ATOM	1380	CB TYR 1 693	-0.396	17.808	-1.809	1.00	1.13
ATOM	1381	CG TYR 1 693	-1.845	17.808	-2.157	1.00	1.13

198/208

ATOM	1382	CD1 TYR 1 693	-2.271	18.338	-3.348	1.00	1.13
ATOM	1383	CD2 TYR 1 693	-2.785	17.299	-1.293	1.00	1.13
ATOM	1384	CE1 TYR 1 693	-3.600	18.367	-3.687	1.00	1.13
ATOM	1385	CE2 TYR 1 693	-4.123	17.333	-1.616	1.00	1.13
ATOM	1386	CZ TYR 1 693	-4.532	17.869	-2.814	1.00	1.13
ATOM	1387	OH TYR 1 693	-5.904	17.965	-3.131	1.00	1.13
ATOM	1388	N ILE 1 694	2.381	19.263	-1.426	1.00	0.61
ATOM	1389	CA ILE 1 694	3.674	19.185	-0.803	1.00	0.61
ATOM	1390	C ILE 1 694	3.869	20.332	0.139	1.00	0.61
ATOM	1391	O ILE 1 694	4.382	20.153	1.244	1.00	0.61
ATOM	1392	CB ILE 1 694	4.797	19.235	-1.797	1.00	0.61
ATOM	1393	CG1 ILE 1 694	4.708	18.050	-2.772	1.00	0.61
ATOM	1394	CG2 ILE 1 694	6.121	19.294	-1.016	1.00	0.61
ATOM	1395	CD1 ILE 1 694	5.631	18.187	-3.983	1.00	0.61
ATOM	1396	N LYS 1 695	3.463	21.547	-0.271	1.00	8.13
ATOM	1397	CA LYS 1 695	3.654	22.702	0.559	1.00	8.13
ATOM	1398	C LYS 1 695	2.868	22.556	1.822	1.00	8.13
ATOM	1399	O LYS 1 695	3.366	22.835	2.912	1.00	8.13
ATOM	1400	CB LYS 1 695	3.189	23.998	-0.126	1.00	8.13
ATOM	1401	CG LYS 1 695	3.567	25.267	0.640	1.00	8.13
ATOM	1402	CD LYS 1 695	5.066	25.573	0.615	1.00	8.13
ATOM	1403	CE LYS 1 695	5.917	24.542	1.359	1.00	8.13
ATOM	1404	NZ LYS 1 695	5.642	24.610	2.811	1.00	8.13
ATOM	1405	N GLU 1 696	1.609	22.098	1.705	1.00	1.25
ATOM	1406	CA GLU 1 696	0.766	21.945	2.853	1.00	1.25
ATOM	1407	C GLU 1 696	1.349	20.908	3.750	1.00	1.25
ATOM	1408	O GLU 1 696	1.299	21.027	4.973	1.00	1.25
ATOM	1409	CB GLU 1 696	-0.655	21.486	2.498	1.00	1.25
ATOM	1410	CG GLU 1 696	-1.425	22.546	1.722	1.00	1.25
ATOM	1411	CD GLU 1 696	-2.816	22.018	1.423	1.00	1.25
ATOM	1412	OE1 GLU 1 696	-3.532	22.684	0.629	1.00	1.25
ATOM	1413	OE2 GLU 1 696	-3.181	20.951	1.982	1.00	1.25
ATOM	1414	N LEU 1 697	1.913	19.842	3.161	1.00	8.40
ATOM	1415	CA LEU 1 697	2.441	18.787	3.970	1.00	8.40
ATOM	1416	C LEU 1 697	3.586	19.306	4.776	1.00	8.40
ATOM	1417	O LEU 1 697	3.701	19.017	5.967	1.00	8.40
ATOM	1418	CB LEU 1 697	2.977	17.603	3.151	1.00	8.40
ATOM	1419	CG LEU 1 697	1.981	17.123	2.084	1.00	8.40
ATOM	1420	CD1 LEU 1 697	2.257	15.678	1.640	1.00	8.40
ATOM	1421	CD2 LEU 1 697	0.530	17.468	2.462	1.00	8.40
ATOM	1422	N GLY 1 698	4.466	20.103	4.143	1.00	0.45
ATOM	1423	CA GLY 1 698	5.622	20.592	4.835	1.00	0.45
ATOM	1424	C GLY 1 698	5.201	21.455	5.979	1.00	0.45
ATOM	1425	O GLY 1 698	5.741	21.351	7.080	1.00	0.45
ATOM	1426	N LYS 1 699	4.211	22.333	5.748	1.00	5.59
ATOM	1427	CA LYS 1 699	3.791	23.224	6.787	1.00	5.59
ATOM	1428	C LYS 1 699	3.230	22.419	7.911	1.00	5.59
ATOM	1429	O LYS 1 699	3.441	22.737	9.079	1.00	5.59
ATOM	1430	CB LYS 1 699	2.680	24.193	6.357	1.00	5.59
ATOM	1431	CG LYS 1 699	1.342	23.489	6.155	1.00	5.59
ATOM	1432	CD LYS 1 699	0.150	24.428	6.129	1.00	5.59
ATOM	1433	CE LYS 1 699	0.256	25.462	5.020	1.00	5.59
ATOM	1434	NZ LYS 1 699	-0.767	26.488	5.248	1.00	5.59
ATOM	1435	N ALA 1 700	2.489	21.346	7.580	1.00	0.65
ATOM	1436	CA ALA 1 700	1.876	20.550	8.598	1.00	0.65
ATOM	1437	C ALA 1 700	2.941	19.933	9.443	1.00	0.65
ATOM	1438	O ALA 1 700	2.831	19.901	10.667	1.00	0.65
ATOM	1439	CB ALA 1 700	1.015	19.412	8.026	1.00	0.65
ATOM	1440	N ILE 1 701	4.017	19.433	8.810	1.00	3.82
ATOM	1441	CA ILE 1 701	5.036	18.790	9.585	1.00	3.82
ATOM	1442	C ILE 1 701	5.693	19.794	10.475	1.00	3.82



199/208

ATOM 1443 O ILE 1 701	6.075	19.481	11.602	1.00	3.82
ATOM 1444 CB ILE 1 701	6.075	18.082	8.764	1.00	3.82
ATOM 1445 CG1 ILE 1 701	6.839	17.095	9.659	1.00	3.82
ATOM 1446 CG2 ILE 1 701	6.979	19.119	8.079	1.00	3.82
ATOM 1447 CD1 ILE 1 701	7.626	16.051	8.874	1.00	3.82
ATOM 1448 N VAL 1 702	5.845	21.039	9.986	1.00	0.51
ATOM 1449 CA VAL 1 702	6.428	22.062	10.798	1.00	0.51
ATOM 1450 C VAL 1 702	5.517	22.229	11.968	1.00	0.51
ATOM 1451 O VAL 1 702	5.964	22.385	13.104	1.00	0.51
ATOM 1452 CB VAL 1 702	6.515	23.385	10.096	1.00	0.51
ATOM 1453 CG1 VAL 1 702	7.095	24.420	11.074	1.00	0.51
ATOM 1454 CG2 VAL 1 702	7.344	23.206	8.812	1.00	0.51
ATOM 1455 N LYS 1 703	4.197	22.165	11.712	1.00	9.37
ATOM 1456 CA LYS 1 703	3.230	22.326	12.756	1.00	9.37
ATOM 1457 C LYS 1 703	3.514	21.258	13.752	1.00	9.37
ATOM 1458 O LYS 1 703	3.431	21.497	14.955	1.00	9.37
ATOM 1459 CB LYS 1 703	1.780	22.143	12.269	1.00	9.37
ATOM 1460 CG LYS 1 703	0.715	22.521	13.305	1.00	9.37
ATOM 1461 CD LYS 1 703	0.716	21.657	14.570	1.00	9.37
ATOM 1462 CE LYS 1 703	0.197	20.237	14.342	1.00	9.37
ATOM 1463 NZ LYS 1 703	-1.226	20.280	13.937	1.00	9.37
ATOM 1464 N ARG 1 704	3.839	20.043	13.267	1.00	8.04
ATOM 1465 CA ARG 1 704	4.206	18.988	14.163	1.00	8.04
ATOM 1466 C ARG 1 704	5.501	19.453	14.723	1.00	8.04
ATOM 1467 O ARG 1 704	6.557	19.224	14.134	1.00	8.04
ATOM 1468 CB ARG 1 704	4.479	17.646	13.467	1.00	8.04
ATOM 1469 CG ARG 1 704	3.235	17.002	12.861	1.00	8.04
ATOM 1470 CD ARG 1 704	2.385	16.248	13.882	1.00	8.04
ATOM 1471 NE ARG 1 704	1.223	15.686	13.146	1.00	8.04
ATOM 1472 CZ ARG 1 704	0.363	14.832	13.771	1.00	8.04
ATOM 1473 NH1 ARG 1 704	0.560	14.486	15.077	1.00	8.04
ATOM 1474 NH2 ARG 1 704	-0.703	14.331	13.084	1.00	8.04
ATOM 1475 N GLU 1 705	5.433	20.112	15.891	1.00	6.89
ATOM 1476 CA GLU 1 705	6.571	20.722	16.502	1.00	6.89
ATOM 1477 C GLU 1 705	7.717	19.793	16.543	1.00	6.89
ATOM 1478 O GLU 1 705	7.541	18.584	16.667	1.00	6.89
ATOM 1479 CB GLU 1 705	6.312	21.210	17.939	1.00	6.89
ATOM 1480 CG GLU 1 705	5.415	22.446	18.000	1.00	6.89
ATOM 1481 CD GLU 1 705	6.174	23.576	17.320	1.00	6.89
ATOM 1482 OE1 GLU 1 705	5.603	24.693	17.201	1.00	6.89
ATOM 1483 OE2 GLU 1 705	7.339	23.332	16.906	1.00	6.89
ATOM 1484 N GLY 1 706	8.927	20.362	16.413	1.00	2.21
ATOM 1485 CA GLY 1 706	10.141	19.610	16.420	1.00	2.21
ATOM 1486 C GLY 1 706	10.330	19.086	17.800	1.00	2.21
ATOM 1487 O GLY 1 706	11.162	18.208	18.022	1.00	2.21
ATOM 1488 N ASN 1 707	9.576	19.640	18.769	1.00	3.74
ATOM 1489 CA ASN 1 707	9.717	19.183	20.118	1.00	3.74
ATOM 1490 C ASN 1 707	9.444	17.717	20.094	1.00	3.74
ATOM 1491 O ASN 1 707	10.295	16.908	20.458	1.00	3.74
ATOM 1492 CB ASN 1 707	8.712	19.832	21.086	1.00	3.74
ATOM 1493 CG ASN 1 707	9.135	19.488	22.509	1.00	3.74
ATOM 1494 OD1 ASN 1 707	8.484	19.885	23.475	1.00	3.74
ATOM 1495 ND2 ASN 1 707	10.260	18.739	22.647	1.00	3.74
ATOM 1496 N SER 1 708	8.238	17.327	19.649	1.00	3.07
ATOM 1497 CA SER 1 708	7.976	15.927	19.536	1.00	3.07
ATOM 1498 C SER 1 708	8.722	15.483	18.319	1.00	3.07
ATOM 1499 O SER 1 708	9.414	14.466	18.325	1.00	3.07
ATOM 1500 CB SER 1 708	6.487	15.607	19.324	1.00	3.07
ATOM 1501 OG SER 1 708	6.299	14.204	19.220	1.00	3.07
ATOM 1502 N SER 1 709	8.607	16.282	17.242	1.00	4.34
ATOM 1503 CA SER 1 709	9.228	15.993	15.988	1.00	4.34

200/208

ATOM	1504	C	SER	1709	10.693	16.280	16.079	1.00	4.34
ATOM	1505	O	SER	1709	11.242	16.982	15.230	1.00	4.34
ATOM	1506	CB	SER	1709	8.652	16.859	14.853	1.00	4.34
ATOM	1507	OG	SER	1709	9.278	16.563	13.617	1.00	4.34
ATOM	1508	N	GLN	1710	11.389	15.761	17.111	1.00	3.96
ATOM	1509	CA	GLN	1710	12.803	15.981	17.041	1.00	3.96
ATOM	1510	C	GLN	1710	13.402	14.857	16.284	1.00	3.96
ATOM	1511	O	GLN	1710	13.900	13.888	16.857	1.00	3.96
ATOM	1512	CB	GLN	1710	13.607	16.084	18.355	1.00	3.96
ATOM	1513	CG	GLN	1710	13.732	17.498	18.931	1.00	3.96
ATOM	1514	CD	GLN	1710	12.928	17.617	20.209	1.00	3.96
ATOM	1515	OE1	GLN	1710	12.380	18.674	20.514	1.00	3.96
ATOM	1516	NE2	GLN	1710	12.875	16.511	20.998	1.00	3.96
ATOM	1517	N	ASN	1711	13.342	14.967	14.951	1.00	4.08
ATOM	1518	CA	ASN	1711	13.976	14.014	14.103	1.00	4.08
ATOM	1519	C	ASN	1711	14.772	14.907	13.220	1.00	4.08
ATOM	1520	O	ASN	1711	14.246	15.879	12.682	1.00	4.08
ATOM	1521	CB	ASN	1711	12.996	13.224	13.218	1.00	4.08
ATOM	1522	CG	ASN	1711	13.739	12.049	12.597	1.00	4.08
ATOM	1523	OD1	ASN	1711	13.346	10.895	12.759	1.00	4.08
ATOM	1524	ND2	ASN	1711	14.845	12.343	11.864	1.00	4.08
ATOM	1525	N	TRP	1712	16.076	14.630	13.069	1.00	4.56
ATOM	1526	CA	TRP	1712	16.846	15.510	12.249	1.00	4.56
ATOM	1527	C	TRP	1712	16.558	15.188	10.823	1.00	4.56
ATOM	1528	O	TRP	1712	16.349	14.030	10.466	1.00	4.56
ATOM	1529	CB	TRP	1712	18.366	15.377	12.449	1.00	4.56
ATOM	1530	CG	TRP	1712	18.903	13.991	12.181	1.00	4.56
ATOM	1531	CD1	TRP	1712	19.096	13.350	10.992	1.00	4.56
ATOM	1532	CD2	TRP	1712	19.394	13.108	13.202	1.00	4.56
ATOM	1533	NE1	TRP	1712	19.650	12.111	11.211	1.00	4.56
ATOM	1534	CE2	TRP	1712	19.844	11.952	12.567	1.00	4.56
ATOM	1535	CE3	TRP	1712	19.471	13.253	14.559	1.00	4.56
ATOM	1536	CZ2	TRP	1712	20.375	10.915	13.280	1.00	4.56
ATOM	1537	CZ3	TRP	1712	20.010	12.208	15.275	1.00	4.56
ATOM	1538	CH2	TRP	1712	20.452	11.061	14.648	1.00	4.56
ATOM	1539	N	GLN	1713	16.527	16.223	9.966	1.00	4.63
ATOM	1540	CA	GLN	1713	16.349	15.980	8.566	1.00	4.63
ATOM	1541	C	GLN	1713	14.980	15.395	8.370	1.00	4.63
ATOM	1542	O	GLN	1713	14.782	14.579	7.474	1.00	4.63
ATOM	1543	CB	GLN	1713	17.343	14.909	8.068	1.00	4.63
ATOM	1544	CG	GLN	1713	18.778	15.071	8.596	1.00	4.63
ATOM	1545	CD	GLN	1713	19.638	15.895	7.648	1.00	4.63
ATOM	1546	OE1	GLN	1713	19.889	15.497	6.512	1.00	4.63
ATOM	1547	NE2	GLN	1713	20.121	17.070	8.134	1.00	4.63
ATOM	1548	N	ARG	1714	13.987	15.802	9.188	1.00	3.83
ATOM	1549	CA	ARG	1714	12.701	15.167	9.100	1.00	3.83
ATOM	1550	C	ARG	1714	11.971	15.323	7.801	1.00	3.83
ATOM	1551	O	ARG	1714	11.537	14.331	7.218	1.00	3.83
ATOM	1552	CB	ARG	1714	11.716	15.608	10.193	1.00	3.83
ATOM	1553	CG	ARG	1714	10.353	14.928	10.041	1.00	3.83
ATOM	1554	CD	ARG	1714	9.426	15.134	11.235	1.00	3.83
ATOM	1555	NE	ARG	1714	9.949	14.285	12.341	1.00	3.83
ATOM	1556	CZ	ARG	1714	9.284	13.149	12.699	1.00	3.83
ATOM	1557	NH1	ARG	1714	9.786	12.343	13.678	1.00	3.83
ATOM	1558	NH2	ARG	1714	8.109	12.828	12.083	1.00	3.83
ATOM	1559	N	PHE	1715	11.811	16.556	7.285	1.00	7.35
ATOM	1560	CA	PHE	1715	10.994	16.649	6.108	1.00	7.35
ATOM	1561	C	PHE	1715	11.615	15.939	4.948	1.00	7.35
ATOM	1562	O	PHE	1715	10.968	15.128	4.287	1.00	7.35
ATOM	1563	CB	PHE	1715	10.643	18.095	5.701	1.00	7.35
ATOM	1564	CG	PHE	1715	11.864	18.861	5.318	1.00	7.35

201/208

ATOM	1565	CD1 PHE 1 715	12.296	18.874	4.011	1.00	7.35
ATOM	1566	CD2 PHE 1 715	12.497	19.665	6.236	1.00	7.35
ATOM	1567	CE1 PHE 1 715	13.350	19.671	3.630	1.00	7.35
ATOM	1568	CE2 PHE 1 715	13.555	20.459	5.862	1.00	7.35
ATOM	1569	CZ PHE 1 715	13.977	20.472	4.554	1.00	7.35
ATOM	1570	N TYR 1 716	12.905	16.199	4.687	1.00	4.17
ATOM	1571	CA TYR 1 716	13.554	15.554	3.588	1.00	4.17
ATOM	1572	C TYR 1 716	13.721	14.089	3.821	1.00	4.17
ATOM	1573	O TYR 1 716	13.701	13.300	2.878	1.00	4.17
ATOM	1574	CB TYR 1 716	14.874	16.225	3.162	1.00	4.17
ATOM	1575	CG TYR 1 716	15.608	16.683	4.370	1.00	4.17
ATOM	1576	CD1 TYR 1 716	15.188	17.824	5.012	1.00	4.17
ATOM	1577	CD2 TYR 1 716	16.814	16.131	4.723	1.00	4.17
ATOM	1578	CE1 TYR 1 716	15.914	18.386	6.031	1.00	4.17
ATOM	1579	CE2 TYR 1 716	17.552	16.698	5.733	1.00	4.17
ATOM	1580	CZ TYR 1 716	17.109	17.820	6.391	1.00	4.17
ATOM	1581	OH TYR 1 716	17.871	18.391	7.430	1.00	4.17
ATOM	1582	N GLN 1 717	13.892	13.661	5.083	1.00	4.45
ATOM	1583	CA GLN 1 717	14.034	12.252	5.290	1.00	4.45
ATOM	1584	C GLN 1 717	12.760	11.597	4.856	1.00	4.45
ATOM	1585	O GLN 1 717	12.790	10.543	4.227	1.00	4.45
ATOM	1586	CB GLN 1 717	14.289	11.853	6.756	1.00	4.45
ATOM	1587	CG GLN 1 717	13.128	12.151	7.705	1.00	4.45
ATOM	1588	CD GLN 1 717	13.537	11.704	9.101	1.00	4.45
ATOM	1589	OE1 GLN 1 717	12.744	11.748	10.041	1.00	4.45
ATOM	1590	NE2 GLN 1 717	14.812	11.253	9.242	1.00	4.45
ATOM	1591	N LEU 1 718	11.612	12.225	5.182	1.00	0.89
ATOM	1592	CA LEU 1 718	10.315	11.703	4.853	1.00	0.89
ATOM	1593	C LEU 1 718	10.116	11.696	3.366	1.00	0.89
ATOM	1594	O LEU 1 718	9.529	10.760	2.823	1.00	0.89
ATOM	1595	CB LEU 1 718	9.173	12.524	5.478	1.00	0.89
ATOM	1596	CG LEU 1 718	7.772	11.987	5.137	1.00	0.89
ATOM	1597	CD1 LEU 1 718	7.570	10.569	5.700	1.00	0.89
ATOM	1598	CD2 LEU 1 718	6.674	12.963	5.589	1.00	0.89
ATOM	1599	N THR 1 719	10.607	12.736	2.666	1.00	4.49
ATOM	1600	CA THR 1 719	10.417	12.802	1.244	1.00	4.49
ATOM	1601	C THR 1 719	11.120	11.627	0.650	1.00	4.49
ATOM	1602	O THR 1 719	10.716	11.101	-0.385	1.00	4.49
ATOM	1603	CB THR 1 719	10.957	14.047	0.599	1.00	4.49
ATOM	1604	OG1 THR 1 719	10.426	14.178	-0.712	1.00	4.49
ATOM	1605	CG2 THR 1 719	12.487	13.952	0.516	1.00	4.49
ATOM	1606	N LYS 1 720	12.203	11.191	1.313	1.00	8.13
ATOM	1607	CA LYS 1 720	12.989	10.077	0.874	1.00	8.13
ATOM	1608	C LYS 1 720	12.109	8.864	0.840	1.00	8.13
ATOM	1609	O LYS 1 720	12.278	7.996	-0.013	1.00	8.13
ATOM	1610	CB LYS 1 720	14.177	9.812	1.819	1.00	8.13
ATOM	1611	CG LYS 1 720	15.149	8.724	1.356	1.00	8.13
ATOM	1612	CD LYS 1 720	14.561	7.313	1.350	1.00	8.13
ATOM	1613	CE LYS 1 720	14.315	6.750	2.752	1.00	8.13
ATOM	1614	NZ LYS 1 720	13.746	5.387	2.658	1.00	8.13
ATOM	1615	N LEU 1 721	11.139	8.777	1.770	1.00	3.53
ATOM	1616	CA LEU 1 721	10.246	7.652	1.836	1.00	3.53
ATOM	1617	C LEU 1 721	9.467	7.564	0.564	1.00	3.53
ATOM	1618	O LEU 1 721	9.163	6.476	0.080	1.00	3.53
ATOM	1619	CB LEU 1 721	9.203	7.760	2.965	1.00	3.53
ATOM	1620	CG LEU 1 721	9.775	7.642	4.388	1.00	3.53
ATOM	1621	CD1 LEU 1 721	10.758	8.774	4.697	1.00	3.53
ATOM	1622	CD2 LEU 1 721	8.647	7.568	5.426	1.00	3.53
ATOM	1623	N LEU 1 722	9.113	8.720	-0.014	1.00	4.47
ATOM	1624	CA LEU 1 722	8.339	8.721	-1.217	1.00	4.47
ATOM	1625	C LEU 1 722	9.128	7.983	-2.250	1.00	4.47

202/208

ATOM	1626	O	LEU	1	722	8.576	7.213	-3.035	1.00	4.47
ATOM	1627	CB	LEU	1	722	8.075	10.143	-1.733	1.00	4.47
ATOM	1628	CG	LEU	1	722	7.237	10.990	-0.759	1.00	4.47
ATOM	1629	CD1	LEU	1	722	7.970	11.234	0.569	1.00	4.47
ATOM	1630	CD2	LEU	1	722	6.785	12.297	-1.417	1.00	4.47
ATOM	1631	N	ASP	1	723	10.455	8.197	-2.256	1.00	4.04
ATOM	1632	CA	ASP	1	723	11.333	7.563	-3.195	1.00	4.04
ATOM	1633	C	ASP	1	723	11.247	6.081	-3.008	1.00	4.04
ATOM	1634	O	ASP	1	723	11.102	5.331	-3.973	1.00	4.04
ATOM	1635	CB	ASP	1	723	12.801	7.981	-2.965	1.00	4.04
ATOM	1636	CG	ASP	1	723	13.697	7.406	-4.055	1.00	4.04
ATOM	1637	OD1	ASP	1	723	14.413	8.214	-4.705	1.00	4.04
ATOM	1638	OD2	ASP	1	723	13.684	6.163	-4.258	1.00	4.04
ATOM	1639	N	SER	1	724	11.308	5.619	-1.747	1.00	3.24
ATOM	1640	CA	SER	1	724	11.287	4.209	-1.498	1.00	3.24
ATOM	1641	C	SER	1	724	9.986	3.653	-1.977	1.00	3.24
ATOM	1642	O	SER	1	724	9.938	2.558	-2.534	1.00	3.24
ATOM	1643	CB	SER	1	724	11.446	3.845	-0.009	1.00	3.24
ATOM	1644	OG	SER	1	724	10.310	4.264	0.732	1.00	3.24
ATOM	1645	N	MET	1	725	8.890	4.407	-1.776	1.00	0.77
ATOM	1646	CA	MET	1	725	7.590	3.949	-2.165	1.00	0.77
ATOM	1647	C	MET	1	725	7.516	3.774	-3.652	1.00	0.77
ATOM	1648	O	MET	1	725	6.920	2.815	-4.138	1.00	0.77
ATOM	1649	CB	MET	1	725	6.465	4.916	-1.756	1.00	0.77
ATOM	1650	CG	MET	1	725	6.331	5.076	-0.241	1.00	0.77
ATOM	1651	SD	MET	1	725	4.967	6.152	0.289	1.00	0.77
ATOM	1652	CE	MET	1	725	3.672	4.931	-0.072	1.00	0.77
ATOM	1653	N	HIS	1	726	8.098	4.697	-4.438	1.00	3.69
ATOM	1654	CA	HIS	1	726	8.018	4.491	-5.855	1.00	3.69
ATOM	1655	C	HIS	1	726	8.835	3.300	-6.224	1.00	3.69
ATOM	1656	O	HIS	1	726	8.536	2.585	-7.177	1.00	3.69
ATOM	1657	CB	HIS	1	726	8.434	5.689	-6.730	1.00	3.69
ATOM	1658	CG	HIS	1	726	9.861	6.124	-6.617	1.00	3.69
ATOM	1659	ND1	HIS	1	726	10.251	7.298	-6.014	1.00	3.69
ATOM	1660	CD2	HIS	1	726	10.990	5.583	-7.148	1.00	3.69
ATOM	1661	CE1	HIS	1	726	11.586	7.412	-6.215	1.00	3.69
ATOM	1662	NE2	HIS	1	726	12.083	6.392	-6.892	1.00	3.69
ATOM	1663	N	GLU	1	727	9.922	3.054	-5.483	1.00	3.10
ATOM	1664	CA	GLU	1	727	10.722	1.912	-5.796	1.00	3.10
ATOM	1665	C	GLU	1	727	9.893	0.682	-5.611	1.00	3.10
ATOM	1666	O	GLU	1	727	9.911	-0.216	-6.453	1.00	3.10
ATOM	1667	CB	GLU	1	727	11.945	1.794	-4.872	1.00	3.10
ATOM	1668	CG	GLU	1	727	12.968	2.911	-5.081	1.00	3.10
ATOM	1669	CD	GLU	1	727	13.728	2.599	-6.360	1.00	3.10
ATOM	1670	OE1	GLU	1	727	14.682	3.355	-6.684	1.00	3.10
ATOM	1671	OE2	GLU	1	727	13.365	1.595	-7.029	1.00	3.10
ATOM	1672	N	VAL	1	728	9.116	0.615	-4.512	1.00	3.54
ATOM	1673	CA	VAL	1	728	8.362	-0.578	-4.262	1.00	3.54
ATOM	1674	C	VAL	1	728	7.337	-0.786	-5.333	1.00	3.54
ATOM	1675	O	VAL	1	728	7.119	-1.913	-5.772	1.00	3.54
ATOM	1676	CB	VAL	1	728	7.677	-0.623	-2.919	1.00	3.54
ATOM	1677	CG1	VAL	1	728	8.755	-0.522	-1.828	1.00	3.54
ATOM	1678	CG2	VAL	1	728	6.576	0.440	-2.837	1.00	3.54
ATOM	1679	N	VAL	1	729	6.684	0.294	-5.803	1.00	3.39
ATOM	1680	CA	VAL	1	729	5.675	0.117	-6.810	1.00	3.39
ATOM	1681	C	VAL	1	729	6.279	-0.428	-8.067	1.00	3.39
ATOM	1682	O	VAL	1	729	5.694	-1.291	-8.720	1.00	3.39
ATOM	1683	CB	VAL	1	729	4.943	1.375	-7.186	1.00	3.39
ATOM	1684	CG1	VAL	1	729	5.919	2.329	-7.879	1.00	3.39
ATOM	1685	CG2	VAL	1	729	3.762	1.002	-8.099	1.00	3.39
ATOM	1686	N	GLU	1	730	7.477	0.063	-8.441	1.00	1.12

203/208

ATOM	1687	CA	GLU	1	730	8.090	-0.357	-9.663	1.00	1.12
ATOM	1688	C	GLU	1	730	8.377	-1.815	-9.564	1.00	1.12
ATOM	1689	O	GLU	1	730	8.113	-2.579	-10.490	1.00	1.12
ATOM	1690	CB	GLU	1	730	9.431	0.350	-9.936	1.00	1.12
ATOM	1691	CG	GLU	1	730	9.310	1.849	-10.229	1.00	1.12
ATOM	1692	CD	GLU	1	730	10.714	2.390	-10.474	1.00	1.12
ATOM	1693	OE1	GLU	1	730	10.842	3.618	-10.731	1.00	1.12
ATOM	1694	OE2	GLU	1	730	11.680	1.583	-10.410	1.00	1.12
ATOM	1695	N	ASN	1	731	8.908	-2.238	-8.405	1.00	3.09
ATOM	1696	CA	ASN	1	731	9.277	-3.607	-8.203	1.00	3.09
ATOM	1697	C	ASN	1	731	8.062	-4.472	-8.272	1.00	3.09
ATOM	1698	O	ASN	1	731	8.100	-5.581	-8.801	1.00	3.09
ATOM	1699	CB	ASN	1	731	9.937	-3.838	-6.836	1.00	3.09
ATOM	1700	CG	ASN	1	731	10.529	-5.236	-6.849	1.00	3.09
ATOM	1701	OD1	ASN	1	731	9.829	-6.227	-7.053	1.00	3.09
ATOM	1702	ND2	ASN	1	731	11.870	-5.318	-6.641	1.00	3.09
ATOM	1703	N	LEU	1	732	6.935	-3.981	-7.738	1.00	1.26
ATOM	1704	CA	LEU	1	732	5.742	-4.771	-7.713	1.00	1.26
ATOM	1705	C	LEU	1	732	5.349	-5.051	-9.132	1.00	1.26
ATOM	1706	O	LEU	1	732	4.895	-6.146	-9.456	1.00	1.26
ATOM	1707	CB	LEU	1	732	4.593	-4.049	-6.971	1.00	1.26
ATOM	1708	CG	LEU	1	732	3.312	-4.871	-6.685	1.00	1.26
ATOM	1709	CD1	LEU	1	732	2.279	-4.010	-5.941	1.00	1.26
ATOM	1710	CD2	LEU	1	732	2.700	-5.502	-7.945	1.00	1.26
ATOM	1711	N	LEU	1	733	5.537	-4.073	-10.034	1.00	6.33
ATOM	1712	CA	LEU	1	733	5.142	-4.289	-11.394	1.00	6.33
ATOM	1713	C	LEU	1	733	5.868	-5.480	-11.943	1.00	6.33
ATOM	1714	O	LEU	1	733	5.287	-6.307	-12.642	1.00	6.33
ATOM	1715	CB	LEU	1	733	5.480	-3.096	-12.307	1.00	6.33
ATOM	1716	CG	LEU	1	733	5.063	-3.298	-13.777	1.00	6.33
ATOM	1717	CD1	LEU	1	733	3.536	-3.380	-13.924	1.00	6.33
ATOM	1718	CD2	LEU	1	733	5.696	-2.234	-14.689	1.00	6.33
ATOM	1719	N	ASN	1	734	7.172	-5.615	-11.663	1.00	4.20
ATOM	1720	CA	ASN	1	734	7.856	-6.750	-12.213	1.00	4.20
ATOM	1721	C	ASN	1	734	7.377	-8.043	-11.629	1.00	4.20
ATOM	1722	O	ASN	1	734	7.196	-9.035	-12.335	1.00	4.20
ATOM	1723	CB	ASN	1	734	9.398	-6.679	-12.092	1.00	4.20
ATOM	1724	CG	ASN	1	734	9.854	-6.616	-10.639	1.00	4.20
ATOM	1725	OD1	ASN	1	734	10.239	-5.552	-10.159	1.00	4.20
ATOM	1726	ND2	ASN	1	734	9.831	-7.775	-9.927	1.00	4.20
ATOM	1727	N	TYR	1	735	7.136	-8.093	-10.314	1.00	7.65
ATOM	1728	CA	TYR	1	735	6.749	-9.366	-9.802	1.00	7.65
ATOM	1729	C	TYR	1	735	5.394	-9.717	-10.306	1.00	7.65
ATOM	1730	O	TYR	1	735	5.118	-10.881	-10.597	1.00	7.65
ATOM	1731	CB	TYR	1	735	6.652	-9.443	-8.283	1.00	7.65
ATOM	1732	CG	TYR	1	735	6.449	-10.889	-7.992	1.00	7.65
ATOM	1733	CD1	TYR	1	735	7.537	-11.677	-7.696	1.00	7.65
ATOM	1734	CD2	TYR	1	735	5.188	-11.455	-7.945	1.00	7.65
ATOM	1735	CE1	TYR	1	735	7.377	-12.989	-7.317	1.00	7.65
ATOM	1736	CE2	TYR	1	735	5.026	-12.770	-7.578	1.00	7.65
ATOM	1737	CZ	TYR	1	735	6.118	-13.531	-7.238	1.00	7.65
ATOM	1738	OH	TYR	1	735	5.951	-14.875	-6.842	1.00	7.65
ATOM	1739	N	CYS	1	736	4.507	-8.714	-10.433	1.00	4.30
ATOM	1740	CA	CYS	1	736	3.158	-9.054	-10.756	1.00	4.30
ATOM	1741	C	CYS	1	736	3.081	-9.771	-12.053	1.00	4.30
ATOM	1742	O	CYS	1	736	2.369	-10.767	-12.164	1.00	4.30
ATOM	1743	CB	CYS	1	736	2.192	-7.856	-10.780	1.00	4.30
ATOM	1744	SG	CYS	1	736	2.518	-6.684	-12.120	1.00	4.30
ATOM	1745	N	PHE	1	737	3.823	-9.323	-13.075	1.00	7.73
ATOM	1746	CA	PHE	1	737	3.655	-10.052	-14.290	1.00	7.73
ATOM	1747	C	PHE	1	737	4.160	-11.453	-14.158	1.00	7.73

204/208

ATOM	1748	O	PHE	1	737	3.507	-12.390	-14.611	1.00	7.73
ATOM	1749	CB	PHE	1	737	4.273	-9.389	-15.540	1.00	7.73
ATOM	1750	CG	PHE	1	737	5.754	-9.302	-15.437	1.00	7.73
ATOM	1751	CD1	PHE	1	737	6.355	-8.226	-14.824	1.00	7.73
ATOM	1752	CD2	PHE	1	737	6.542	-10.220	-16.092	1.00	7.73
ATOM	1753	CE1	PHE	1	737	7.722	-8.082	-14.847	1.00	7.73
ATOM	1754	CE2	PHE	1	737	7.911	-10.092	-16.101	1.00	7.73
ATOM	1755	CZ	PHE	1	737	8.503	-9.023	-15.476	1.00	7.73
ATOM	1756	N	GLN	1	738	5.315	-11.656	-13.493	1.00	7.23
ATOM	1757	CA	GLN	1	738	5.836	-12.990	-13.454	1.00	7.23
ATOM	1758	C	GLN	1	738	4.860	-13.857	-12.729	1.00	7.23
ATOM	1759	O	GLN	1	738	4.605	-14.996	-13.114	1.00	7.23
ATOM	1760	CB	GLN	1	738	7.208	-13.107	-12.762	1.00	7.23
ATOM	1761	CG	GLN	1	738	7.177	-12.981	-11.240	1.00	7.23
ATOM	1762	CD	GLN	1	738	7.120	-14.405	-10.704	1.00	7.23
ATOM	1763	OE1	GLN	1	738	7.186	-14.645	-9.500	1.00	7.23
ATOM	1764	NE2	GLN	1	738	7.013	-15.395	-11.631	1.00	7.23
ATOM	1765	N	THR	1	739	4.283	-13.340	-11.637	1.00	5.24
ATOM	1766	CA	THR	1	739	3.338	-14.132	-10.912	1.00	5.24
ATOM	1767	C	THR	1	739	2.092	-14.330	-11.715	1.00	5.24
ATOM	1768	O	THR	1	739	1.507	-15.413	-11.725	1.00	5.24
ATOM	1769	CB	THR	1	739	2.953	-13.519	-9.596	1.00	5.24
ATOM	1770	OG1	THR	1	739	2.945	-12.102	-9.699	1.00	5.24
ATOM	1771	CG2	THR	1	739	3.949	-13.970	-8.515	1.00	5.24
ATOM	1772	N	PHE	1	740	1.665	-13.276	-12.430	1.00	6.82
ATOM	1773	CA	PHE	1	740	0.434	-13.258	-13.161	1.00	6.82
ATOM	1774	C	PHE	1	740	0.463	-14.242	-14.278	1.00	6.82
ATOM	1775	O	PHE	1	740	-0.558	-14.842	-14.609	1.00	6.82
ATOM	1776	CB	PHE	1	740	0.130	-11.872	-13.756	1.00	6.82
ATOM	1777	CG	PHE	1	740	-1.308	-11.852	-14.142	1.00	6.82
ATOM	1778	CD1	PHE	1	740	-1.724	-12.340	-15.358	1.00	6.82
ATOM	1779	CD2	PHE	1	740	-2.246	-11.343	-13.272	1.00	6.82
ATOM	1780	CE1	PHE	1	740	-3.055	-12.316	-15.701	1.00	6.82
ATOM	1781	CE2	PHE	1	740	-3.577	-11.318	-13.609	1.00	6.82
ATOM	1782	CZ	PHE	1	740	-3.985	-11.804	-14.827	1.00	6.82
ATOM	1783	N	LEU	1	741	1.647	-14.447	-14.877	1.00	5.17
ATOM	1784	CA	LEU	1	741	1.718	-15.298	-16.022	1.00	5.17
ATOM	1785	C	LEU	1	741	1.219	-16.654	-15.648	1.00	5.17
ATOM	1786	O	LEU	1	741	0.458	-17.260	-16.398	1.00	5.17
ATOM	1787	CB	LEU	1	741	3.155	-15.433	-16.573	1.00	5.17
ATOM	1788	CG	LEU	1	741	3.290	-16.235	-17.890	1.00	5.17
ATOM	1789	CD1	LEU	1	741	3.002	-17.735	-17.715	1.00	5.17
ATOM	1790	CD2	LEU	1	741	2.455	-15.594	-19.010	1.00	5.17
ATOM	1791	N	ASP	1	742	1.605	-17.172	-14.469	1.00	6.55
ATOM	1792	CA	ASP	1	742	1.164	-18.507	-14.199	1.00	6.55
ATOM	1793	C	ASP	1	742	0.007	-18.588	-13.252	1.00	6.55
ATOM	1794	O	ASP	1	742	0.168	-18.330	-12.059	1.00	6.55
ATOM	1795	CB	ASP	1	742	2.282	-19.432	-13.678	1.00	6.55
ATOM	1796	CG	ASP	1	742	2.836	-18.875	-12.374	1.00	6.55
ATOM	1797	OD1	ASP	1	742	2.616	-17.665	-12.100	1.00	6.55
ATOM	1798	OD2	ASP	1	742	3.494	-19.654	-11.634	1.00	6.55
ATOM	1799	N	LYS	1	743	-1.188	-18.919	-13.811	1.00	7.11
ATOM	1800	CA	LYS	1	743	-2.427	-19.213	-13.129	1.00	7.11
ATOM	1801	C	LYS	1	743	-3.536	-18.292	-13.532	1.00	7.11
ATOM	1802	O	LYS	1	743	-3.327	-17.101	-13.755	1.00	7.11
ATOM	1803	CB	LYS	1	743	-2.353	-19.214	-11.590	1.00	7.11
ATOM	1804	CG	LYS	1	743	-3.579	-19.800	-10.895	1.00	7.11
ATOM	1805	CD	LYS	1	743	-3.308	-20.161	-9.434	1.00	7.11
ATOM	1806	CE	LYS	1	743	-2.225	-21.231	-9.278	1.00	7.11
ATOM	1807	NZ	LYS	1	743	-2.007	-21.537	-7.847	1.00	7.11
ATOM	1808	N	THR	1	744	-4.764	-18.848	-13.631	1.00	3.77

205/208

ATOM	1809	CA	THR	1744	-5.932	-18.071	-13.934	1.00	3.77
ATOM	1810	C	THR	1744	-6.606	-18.018	-12.601	1.00	3.77
ATOM	1811	O	THR	1744	-5.925	-17.857	-11.590	1.00	3.77
ATOM	1812	CB	THR	1744	-6.839	-18.721	-14.948	1.00	3.77
ATOM	1813	OG1	THR	1744	-6.106	-18.987	-16.136	1.00	3.77
ATOM	1814	CG2	THR	1744	-7.995	-17.762	-15.299	1.00	3.77
ATOM	1815	N	MET	1745	-7.948	-18.136	-12.517	1.00	12.59
ATOM	1816	CA	MET	1745	-8.413	-18.065	-11.172	1.00	12.59
ATOM	1817	C	MET	1745	-9.878	-18.181	-10.986	1.00	12.59
ATOM	1818	O	MET	1745	-10.676	-17.804	-11.842	1.00	12.59
ATOM	1819	CB	MET	1745	-8.183	-16.711	-10.536	1.00	12.59
ATOM	1820	CG	MET	1745	-9.189	-15.659	-11.022	1.00	12.59
ATOM	1821	SD	MET	1745	-9.788	-14.502	-9.750	1.00	12.59
ATOM	1822	CE	MET	1745	-10.941	-13.605	-10.832	1.00	12.59
ATOM	1823	N	SER	1746	-10.262	-18.777	-9.844	1.00	4.73
ATOM	1824	CA	SER	1746	-11.605	-18.590	-9.414	1.00	4.73
ATOM	1825	C	SER	1746	-11.447	-17.285	-8.692	1.00	4.73
ATOM	1826	O	SER	1746	-11.988	-16.252	-9.084	1.00	4.73
ATOM	1827	CB	SER	1746	-12.061	-19.649	-8.395	1.00	4.73
ATOM	1828	OG	SER	1746	-13.407	-19.413	-8.007	1.00	4.73
ATOM	1829	N	ILE	1747	-10.646	-17.343	-7.603	1.00	6.94
ATOM	1830	CA	ILE	1747	-10.266	-16.253	-6.747	1.00	6.94
ATOM	1831	C	ILE	1747	-8.902	-15.708	-7.066	1.00	6.94
ATOM	1832	O	ILE	1747	-8.586	-14.569	-6.729	1.00	6.94
ATOM	1833	CB	ILE	1747	-10.217	-16.660	-5.303	1.00	6.94
ATOM	1834	CG1	ILE	1747	-9.984	-15.428	-4.414	1.00	6.94
ATOM	1835	CG2	ILE	1747	-9.141	-17.749	-5.149	1.00	6.94
ATOM	1836	CD1	ILE	1747	-11.153	-14.445	-4.422	1.00	6.94
ATOM	1837	N	GLU	1748	-8.062	-16.506	-7.750	1.00	5.83
ATOM	1838	CA	GLU	1748	-6.665	-16.191	-7.900	1.00	5.83
ATOM	1839	C	GLU	1748	-6.317	-14.839	-8.467	1.00	5.83
ATOM	1840	O	GLU	1748	-5.542	-14.112	-7.851	1.00	5.83
ATOM	1841	CB	GLU	1748	-5.904	-17.242	-8.728	1.00	5.83
ATOM	1842	CG	GLU	1748	-4.393	-17.188	-8.502	1.00	5.83
ATOM	1843	CD	GLU	1748	-4.115	-17.849	-7.157	1.00	5.83
ATOM	1844	OE1	GLU	1748	-4.360	-19.080	-7.041	1.00	5.83
ATOM	1845	OE2	GLU	1748	-3.656	-17.133	-6.228	1.00	5.83
ATOM	1846	N	PHE	1749	-6.846	-14.431	-9.636	1.00	0.97
ATOM	1847	CA	PHE	1749	-6.471	-13.137	-10.126	1.00	0.97
ATOM	1848	C	PHE	1749	-7.707	-12.328	-10.320	1.00	0.97
ATOM	1849	O	PHE	1749	-8.441	-12.492	-11.293	1.00	0.97
ATOM	1850	CB	PHE	1749	-5.729	-13.184	-11.471	1.00	0.97
ATOM	1851	CG	PHE	1749	-4.441	-13.886	-11.218	1.00	0.97
ATOM	1852	CD1	PHE	1749	-4.391	-15.260	-11.210	1.00	0.97
ATOM	1853	CD2	PHE	1749	-3.294	-13.173	-10.959	1.00	0.97
ATOM	1854	CE1	PHE	1749	-3.209	-15.915	-10.956	1.00	0.97
ATOM	1855	CE2	PHE	1749	-2.109	-13.822	-10.701	1.00	0.97
ATOM	1856	CZ	PHE	1749	-2.066	-15.196	-10.702	1.00	0.97
ATOM	1857	N	PRO	1750	-7.925	-11.440	-9.397	1.00	2.67
ATOM	1858	CA	PRO	1750	-9.095	-10.620	-9.417	1.00	2.67
ATOM	1859	C	PRO	1750	-9.079	-9.888	-10.712	1.00	2.67
ATOM	1860	O	PRO	1750	-7.998	-9.566	-11.200	1.00	2.67
ATOM	1861	CB	PRO	1750	-8.924	-9.612	-8.279	1.00	2.67
ATOM	1862	CG	PRO	1750	-7.545	-9.932	-7.664	1.00	2.67
ATOM	1863	CD	PRO	1750	-6.833	-10.743	-8.759	1.00	2.67
ATOM	1864	N	GLU	1751	-10.261	-9.636	-11.291	1.00	5.68
ATOM	1865	CA	GLU	1751	-10.318	-8.882	-12.502	1.00	5.68
ATOM	1866	C	GLU	1751	-9.848	-7.504	-12.174	1.00	5.68
ATOM	1867	O	GLU	1751	-9.093	-6.895	-12.931	1.00	5.68
ATOM	1868	CB	GLU	1751	-11.743	-8.770	-13.073	1.00	5.68
ATOM	1869	CG	GLU	1751	-12.741	-8.112	-12.116	1.00	5.68

206 / 208

ATOM	1870	CD	GLU	1 751	-13.010	-9.085	-10.976	1.00	5.68
ATOM	1871	OE1	GLU	1 751	-13.346	-10.263	-11.271	1.00	5.68
ATOM	1872	OE2	GLU	1 751	-12.865	-8.669	-9.796	1.00	5.68
ATOM	1873	N	MET	1 752	-10.275	-6.984	-11.009	1.00	5.28
ATOM	1874	CA	MET	1 752	-9.934	-5.644	-10.636	1.00	5.28
ATOM	1875	C	MET	1 752	-8.448	-5.558	-10.471	1.00	5.28
ATOM	1876	O	MET	1 752	-7.819	-4.609	-10.932	1.00	5.28
ATOM	1877	CB	MET	1 752	-10.589	-5.214	-9.312	1.00	5.28
ATOM	1878	CG	MET	1 752	-10.778	-3.701	-9.185	1.00	5.28
ATOM	1879	SD	MET	1 752	-9.265	-2.716	-9.345	1.00	5.28
ATOM	1880	CE	MET	1 752	-10.099	-1.122	-9.091	1.00	5.28
ATOM	1881	N	LEU	1 753	-7.840	-6.568	-9.818	1.00	0.87
ATOM	1882	CA	LEU	1 753	-6.422	-6.511	-9.613	1.00	0.87
ATOM	1883	C	LEU	1 753	-5.745	-6.551	-10.937	1.00	0.87
ATOM	1884	O	LEU	1 753	-4.771	-5.837	-11.174	1.00	0.87
ATOM	1885	CB	LEU	1 753	-5.856	-7.665	-8.770	1.00	0.87
ATOM	1886	CG	LEU	1 753	-4.331	-7.554	-8.569	1.00	0.87
ATOM	1887	CD1	LEU	1 753	-3.962	-6.286	-7.787	1.00	0.87
ATOM	1888	CD2	LEU	1 753	-3.750	-8.831	-7.940	1.00	0.87
ATOM	1889	N	ALA	1 754	-6.263	-7.386	-11.852	1.00	0.70
ATOM	1890	CA	ALA	1 754	-5.656	-7.499	-13.142	1.00	0.70
ATOM	1891	C	ALA	1 754	-5.733	-6.157	-13.790	1.00	0.70
ATOM	1892	O	ALA	1 754	-4.793	-5.720	-14.451	1.00	0.70
ATOM	1893	CB	ALA	1 754	-6.379	-8.501	-14.058	1.00	0.70
ATOM	1894	N	GLU	1 755	-6.866	-5.460	-13.598	1.00	0.95
ATOM	1895	CA	GLU	1 755	-7.066	-4.196	-14.239	1.00	0.95
ATOM	1896	C	GLU	1 755	-6.048	-3.177	-13.824	1.00	0.95
ATOM	1897	O	GLU	1 755	-5.433	-2.531	-14.670	1.00	0.95
ATOM	1898	CB	GLU	1 755	-8.454	-3.608	-13.929	1.00	0.95
ATOM	1899	CG	GLU	1 755	-8.726	-2.270	-14.618	1.00	0.95
ATOM	1900	CD	GLU	1 755	-10.126	-1.824	-14.224	1.00	0.95
ATOM	1901	OE1	GLU	1 755	-11.063	-2.660	-14.328	1.00	0.95
ATOM	1902	OE2	GLU	1 755	-10.279	-0.644	-13.809	1.00	0.95
ATOM	1903	N	ILE	1 756	-5.818	-3.021	-12.508	1.00	3.83
ATOM	1904	CA	ILE	1 756	-4.918	-2.004	-12.037	1.00	3.83
ATOM	1905	C	ILE	1 756	-3.521	-2.272	-12.504	1.00	3.83
ATOM	1906	O	ILE	1 756	-2.818	-1.368	-12.955	1.00	3.83
ATOM	1907	CB	ILE	1 756	-4.874	-1.937	-10.538	1.00	3.83
ATOM	1908	CG1	ILE	1 756	-6.269	-1.620	-9.974	1.00	3.83
ATOM	1909	CG2	ILE	1 756	-3.801	-0.909	-10.142	1.00	3.83
ATOM	1910	CD1	ILE	1 756	-6.827	-0.277	-10.441	1.00	3.83
ATOM	1911	N	ILE	1 757	-3.091	-3.539	-12.384	1.00	4.18
ATOM	1912	CA	ILE	1 757	-1.774	-3.982	-12.742	1.00	4.18
ATOM	1913	C	ILE	1 757	-1.518	-3.958	-14.217	1.00	4.18
ATOM	1914	O	ILE	1 757	-0.435	-3.571	-14.656	1.00	4.18
ATOM	1915	CB	ILE	1 757	-1.535	-5.393	-12.306	1.00	4.18
ATOM	1916	CG1	ILE	1 757	-1.484	-5.491	-10.772	1.00	4.18
ATOM	1917	CG2	ILE	1 757	-0.288	-5.898	-13.036	1.00	4.18
ATOM	1918	CD1	ILE	1 757	-0.364	-4.662	-10.145	1.00	4.18
ATOM	1919	N	THR	1 758	-2.503	-4.397	-15.023	1.00	5.11
ATOM	1920	CA	THR	1 758	-2.304	-4.465	-16.443	1.00	5.11
ATOM	1921	C	THR	1 758	-2.510	-3.111	-17.031	1.00	5.11
ATOM	1922	O	THR	1 758	-2.949	-2.187	-16.349	1.00	5.11
ATOM	1923	CB	THR	1 758	-3.242	-5.403	-17.143	1.00	5.11
ATOM	1924	OG1	THR	1 758	-2.843	-5.575	-18.496	1.00	5.11
ATOM	1925	CG2	THR	1 758	-4.664	-4.819	-17.077	1.00	5.11
ATOM	1926	N	ASN	1 759	-2.176	-2.957	-18.327	1.00	3.12
ATOM	1927	CA	ASN	1 759	-2.329	-1.679	-18.953	1.00	3.12
ATOM	1928	C	ASN	1 759	-3.541	-1.690	-19.823	1.00	3.12
ATOM	1929	O	ASN	1 759	-3.865	-2.695	-20.451	1.00	3.12
ATOM	1930	CB	ASN	1 759	-1.142	-1.282	-19.849	1.00	3.12



207/208

ATOM	1931	CG ASN 1 759	0.054 -0.997 -18.952 1.00 3.12
ATOM	1932	OD1 ASN 1 759	-0.082 -0.389 -17.891 1.00 3.12
ATOM	1933	ND2 ASN 1 759	1.261 -1.451 -19.385 1.00 3.12
ATOM	1934	N GLN 1 760	-4.259 -0.550 -19.855 1.00 5.67
ATOM	1935	CA GLN 1 760	-5.408 -0.424 -20.700 1.00 5.67
ATOM	1936	C GLN 1 760	-5.158 0.765 -21.564 1.00 5.67
ATOM	1937	O GLN 1 760	-4.484 1.710 -21.155 1.00 5.67
ATOM	1938	CB GLN 1 760	-6.726 -0.152 -19.952 1.00 5.67
ATOM	1939	CG GLN 1 760	-7.226 -1.330 -19.115 1.00 5.67
ATOM	1940	CD GLN 1 760	-6.386 -1.415 -17.851 1.00 5.67
ATOM	1941	OE1 GLN 1 760	-5.555 -0.551 -17.573 1.00 5.67
ATOM	1942	NE2 GLN 1 760	-6.616 -2.492 -17.054 1.00 5.67
ATOM	1943	N ILE 1 761	-5.683 0.737 -22.803 1.00 6.58
ATOM	1944	CA ILE 1 761	-5.500 1.858 -23.672 1.00 6.58
ATOM	1945	C ILE 1 761	-6.750 2.723 -23.555 1.00 6.58
ATOM	1946	O ILE 1 761	-6.596 3.935 -23.246 1.00 6.58
ATOM	1947	CB ILE 1 761	-5.312 1.476 -25.115 1.00 6.58
ATOM	1948	CG1 ILE 1 761	-6.544 0.739 -25.669 1.00 6.58
ATOM	1949	CG2 ILE 1 761	-4.010 0.667 -25.220 1.00 6.58
ATOM	1950	CD1 ILE 1 761	-6.531 0.593 -27.189 1.00 6.58
ATOM	1951	OXT ILE 1 761	-7.873 2.190 -23.762 1.00 99.99
TER	1952	ILE 1 761	
HETATM	1953	C1 STR 1	-2.622 -6.967 -0.799 1.00 0.00
HETATM	1954	C2 STR 1	-3.341 -5.965 0.100 1.00 0.05
HETATM	1955	C3 STR 1	-2.352 -5.075 0.821 1.00 0.40
HETATM	1956	C4 STR 1	-1.095 -4.751 0.129 1.00 0.00
HETATM	1957	C5 STR 1	-0.750 -5.273 -1.062 1.00 -0.25
HETATM	1958	C6 STR 1	0.540 -4.815 -1.735 1.00 0.14
HETATM	1959	C7 STR 1	1.328 -6.000 -2.288 1.00 0.00
HETATM	1960	C8 STR 1	0.456 -6.908 -3.164 1.00 0.00
HETATM	1961	C9 STR 1	-0.724 -7.458 -2.322 1.00 0.00
HETATM	1962	C10 STR 1	-1.626 -6.320 -1.778 1.00 0.11
HETATM	1963	C19 STR 1	-2.391 -5.603 -2.902 1.00 0.00
HETATM	1964	C11 STR 1	-1.524 -8.494 -3.148 1.00 0.00
HETATM	1965	C12 STR 1	-0.648 -9.594 -3.770 1.00 0.00
HETATM	1966	C13 STR 1	0.457 -8.988 -4.641 1.00 0.00
HETATM	1967	C14 STR 1	1.275 -8.093 -3.703 1.00 0.00
HETATM	1968	C15 STR 1	2.508 -7.695 -4.513 1.00 0.00
HETATM	1969	C16 STR 1	2.792 -8.947 -5.345 1.00 0.00
HETATM	1970	C17 STR 1	1.625 -9.911 -5.049 1.00 0.05
HETATM	1971	C20 STR 1	1.304 -10.838 -6.220 1.00 0.35
HETATM	1972	C21 STR 1	0.230 -11.885 -6.041 1.00 0.05
HETATM	1973	O104STR 1	-0.778 -11.710 -7.040 1.00 0.00
HETATM	1974	H104STR 1	-1.162 -10.845 -6.954 1.00 0.00
HETATM	1975	O20 STR 1	1.927 -10.786 -7.267 1.00 -0.45
HETATM	1976	C18 STR 1	-0.161 -8.233 -5.840 1.00 0.00
HETATM	1977	O100STR 1	-2.202 -7.806 -4.202 1.00 0.00
HETATM	1978	H100STR 1	-2.698 -8.429 -4.720 1.00 0.00
HETATM	1979	O3 STR 1	-2.598 -4.635 1.939 1.00 -0.45
HETATM	1980	HE2 HE2 2	6.456 -14.046 -4.976 1.00 99.99
CONECT	1953	1954 1962	
CONECT	1954	1953 1955	
CONECT	1955	1954 1956 1979	
CONECT	1956	1955 1957	
CONECT	1957	1956 1958 1962	
CONECT	1958	1957 1959	
CONECT	1959	1958 1960	
CONECT	1960	1959 1961 1967	
CONECT	1961	1960 1962 1964	
CONECT	1962	1953 1957 1961 1963	
CONECT	1963	1962	

208/208

CONNECT 1964 1961 1965 1977  
CONNECT 1965 1964 1966  
CONNECT 1966 1965 1967 1970 1976  
CONNECT 1967 1960 1966 1968  
CONNECT 1968 1967 1969  
CONNECT 1969 1968 1970  
CONNECT 1970 1966 1969 1971  
CONNECT 1971 1970 1972 1975  
CONNECT 1972 1971 1973  
CONNECT 1973 1972 1974  
CONNECT 1974 1973  
CONNECT 1975 1971  
CONNECT 1976 1966  
CONNECT 1977 1964 1978  
CONNECT 1978 1977  
CONNECT 1979 1955  
MASTER 0 0 0 0 0 0 0 0 0 1979 1 27 19  
END

(19) World Intellectual Property Organization  
International Bureau



(43) International Publication Date  
8 September 2000 (08.09.2000)

PCT

(10) International Publication Number  
**WO 00/52050 A3**

- (51) International Patent Classification<sup>7</sup>: **C07K 14/705**
- (21) International Application Number: **PCT/GB00/00727**
- (22) International Filing Date: **1 March 2000 (01.03.2000)**
- (25) Filing Language: **English**
- (26) Publication Language: **English**
- (30) Priority Data:  
9904441.4 **1 March 1999 (01.03.1999)** **GB**  
9909151.4 **22 April 1999 (22.04.1999)** **GB**
- (71) Applicant (*for all designated States except US*): **KARO BIO AB [SE/SE]; Novum, S-141 57 Huddinge (SE).**
- (72) Inventors; and
- (75) Inventors/Applicants (*for US only*): **GILLNER, Mikael [SE/SE]; 6162 Renstiernas Gata 38, S-116 31 Stockholm (SE). GREENIDGE, Paulette [GB/GB]; 63 Vincent Road, Luton, Bedfordshire LU4 9AN (GB).**
- (74) Agents: **BANNERMAN, David, Gardner et al.; Withers & Rogers, Goldings House, 2 Hays Lane, London SE1 2HW (GB).**
- (81) Designated States (*national*): **AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW.**
- (84) Designated States (*regional*): **ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).**
- Published:  
— *With international search report.*
- (88) Date of publication of the international search report:  
**28 December 2000**
- For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.*



**WO 00/52050 A3**

(54) Title: **HOMOLOGY MODELS OF THE GLUCOCORTICOID RECEPTOR**

(57) Abstract: A method of designing a homology model of the ligand binding domain of a glucocorticoid receptor wherein the homology model may be displayed as a three-dimensional image, the method comprising: (i) providing an amino acid sequence and an x-ray crystallographic structure of the ligand binding domain of a thyroid, estrogen or progesterone receptor; (ii) modifying said x-ray crystallographic structure to take account of differences between the amino acid configuration of the ligand binding domains of the glucocorticoid receptor on the one hand and the thyroid, estrogen, or progesterone receptor on the other hand; (iii) verifying the accuracy of the homology model by comparing it with experimentally-determined binding properties of a number of ligands for the glucocorticoid receptor; and (iv) if required modifying the homology model for greater consistency with those binding properties.

# INTERNATIONAL SEARCH REPORT

International Application No

PCT/GB 00/00727

## A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C07K14/705

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)  
IPC 7 G06F C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 98 56812 A (PIKE ASHLEY CHARLES WILLIAM ;BZOZOWSKI ANDRZEJI MAREK (GB); HUBBAR) 17 December 1998 (1998-12-17) page 3, paragraph 1 page 13, paragraph 3 page 28, paragraph 4 claims 13,53,54,56 ---	1-13, 17-20
X	WO 97 21993 A (UNIV CALIFORNIA) 19 June 1997 (1997-06-19) abstract; claims 10-12,23,29-31,38-45 page 3, paragraph 1 page 10, line 19 - line 27 page 29, line 24 -page 30, line 13 --- -/--	1-13, 17-20



Further documents are listed in the continuation of box C.



Patent family members are listed in annex.

### \* Special categories of cited documents:

- \*A\* document defining the general state of the art which is not considered to be of particular relevance
- \*E\* earlier document but published on or after the international filing date
- \*L\* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- \*O\* document referring to an oral disclosure, use, exhibition or other means
- \*P\* document published prior to the international filing date but later than the priority date claimed

\*T\* later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

\*X\* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

\*Y\* document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

\*Z\* document member of the same patent family

Date of the actual completion of the international search

3 August 2000

Date of mailing of the international search report

15.08.00

Name and mailing address of the ISA

European Patent Office, P.B. 5818 Patentlaan 2  
NL - 2280 HV Rijswijk  
Tel. (+31-70) 340-2040, Tx. 31 651 epo nl,  
Fax: (+31-70) 340-3016

Authorized officer

Filloy García, E

## INTERNATIONAL SEARCH REPORT

International Application No

PCT/GB 00/00727

## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	WO 99 50658 A (GREENE GEOFFREY L ;AGARD DAVID A (US); ARCH DEV CORP (US); KUSHNER) 7 October 1999 (1999-10-07) abstract; claims 1-71 ---	1-13, 17-20
P,X	WO 99 26966 A (APRILETTI JAMES W ;FLETTERICK ROBERT J (US); BAXTER JOHN D (US); K) 3 June 1999 (1999-06-03) abstract; claims 8,17,19 page 3, paragraph 1 - paragraph 2 ---	1-13, 17-20
A	ANSTEAD G M ET AL: "The estradiol pharmacophore: Ligand structure-estrogen receptor binding affinity relationships and a model for the receptor binding site" STERIODS: STRUCTURE, FUNCTION, AND REGULATION,US,ELSEVIER SCIENCE PUBLISHERS, NEW YORK, NY, vol. 62, no. 3, 1 March 1997 (1997-03-01), pages 268-303, XP004057108 ISSN: 0039-128X abstract ---	1-13, 17-20
A	R C J RIBEIRO ET AL: "Mechanisms of Thyroid Hormone Action: Insights from X-ray Crystallographic and Functional Studies" RECENT PROGRESS IN HORMONE RESEARCH,US,ACADEMIC PRESS, NEW YORK, NY, vol. 53, no. 53, 1998, pages 351-394-394, XP002101079 ISSN: 0079-9963 abstract page 373, paragraph 4 page 377, paragraph 2 - paragraph 3 ---	1-13, 17-20
A	BRZOZOWSKI A ET AL: "Molecular basis of agonism and antagonism in the oestrogen receptor" NATURE,GB,MACMILLAN JOURNALS LTD. LONDON, no. 389, 16 October 1997 (1997-10-16), pages 753-758, XP002075907 ISSN: 0028-0836 page 757, left-hand column, paragraph 4 -right-hand column, paragraph 2 ---	1-13, 17-20
A	BOURGUET W ET AL: "Crystal structure of the ligand-binding domain of the human nuclear receptor RXR-alpha" NATURE,GB,MACMILLAN JOURNALS LTD. LONDON, no. 375, 1 July 1995 (1995-07-01), pages 377-382, XP002075905 ISSN: 0028-0836 page 379, right-hand column, paragraph 3 -----	1-13, 17-20

# INTERNATIONAL SEARCH REPORT

International application No.  
PCT/GB 00/00727

## Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:  
because they relate to subject matter not required to be searched by this Authority, namely:
2. ☒ Claims Nos.: 14-16  
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:  
see FURTHER INFORMATION sheet PCT/ISA/210
3. ☐ Claims Nos.:  
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

## Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.
- ☐ No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 14-16

Claims 14-16 refer to a glucocorticoid agonist/antagonist without giving a true technical characterisation. Consequently, the scope of said claims is ambiguous and vague. No meaningful search can be carried out for such claims whose wording is, in fact, a mere recitation of the results to be achieved.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

# INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/GB 00/00727

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 9856812 A	17-12-1998	AU 8028998 A EP 0980386 A	30-12-1998 23-02-2000
WO 9721993 A	19-06-1997	AU 1821697 A AU 717743 B CA 2240024 A EP 0873361 A	03-07-1997 30-03-2000 19-06-1997 28-10-1998
WO 9950658 A	07-10-1999	AU 3457199 A AU 5769099 A WO 9960014 A	18-10-1999 06-12-1999 25-11-1999
WO 9926966 A	03-06-1999	AU 1799999 A	15-06-1999